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EVALUATION OF MICRO-MODELS FOR NEAR SURFACE DISPERSION IN RESERVOIRS

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EVALUATION OF MICRO-MODELS FOR NEAR SURFACE DISPERSION IN RESERVOIRS

by

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and
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submitted under
Grant 5 RO1 WP00705-03
Federal Water Pollution Control Administration

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PREFACE

This report is submitted under Grant 5 RO1 WP00705-03 with the Federal Water Pollution Control Administration. The work was originally begun under Grant WP00705-01A1 of the United States Public Health Service and provides for an investigation of mixing and dispersion processes in reservoirs.

The work reported herein involves an evaluation of micro-models for near surface dispersion in reservoirs. Of particular concern is the application of three computational algorithms applicable to dispersion processes in shear flows such as generated by wind stresses.

The authors are grateful to several individuals for their help with the research and with the preparation of this report. Special thanks go to Drs. Earnest F. Gloyna, Walter L. Moore, and Carl W. Morgan and Mr. Al D'Arezzo with whom several thought provoking sessions were held. The authors also wish to acknowledge Drs. Dale E. Walston and Robert E. Lynch for pertinent advice on the mathematics and numerical analysis work contained within this report. Field and laboratory assistance was provided by Messrs. W. A. White and Ed Bruce. Special thanks also go to the Bureau of Engineering Research of The University of Texas for drafting and to Mrs. Gracie Letts for typing the manuscript.

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The financial support of the Federal Water Pollution Control Administration which has made this study possible is also gratefully acknowledged.

ABSTRACT

An evaluation is made of three computational algorithms for the solution of the two dimensional, convective dispersion equation. These models are applicable on a micro-scale to the material transport in shear flows such as found near the surface in water bodies subject to wind stress. The three algorithms correspond to the explicit, implicit, and characteristic methods of solving the conventional parabolic differential equation normally used to represent dispersion processes.

It was found that:

(a) The characteristic method affords the broadest application insofar as range of initial and boundary conditions are concerned. This method best overcomes the traditional restrictions imposed on mathematical solutions and facilitates the construction of representative grid systems with attendant savings in computer processing costs and time.

(b) The explicit method affords practical application for flow situations involving low velocities and diffusion coefficients.

(c) The implicit method has a broader range of practical applications but it is somewhat more complex to program and also more time-consuming to apply. However, this method is the most accurate of the three algorithms.

(d) While each of the micro-models evaluated in this study are not universally applicable to all two dimensional convective dispersion problems, they constitute useful constructs for the analysis of the material transport in near surface, shear flow situations.

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Chapter 1

INTRODUCTION

1-1 Justification

The following study is an outgrowth of problems encountered in deep water storage reservoirs by Wilson and Masch [1967][1] while studying near surface short-term dispersion. These field investigations indicated the expected difficulties, high costs and long time delays involved in obtaining reliable, correlational field data as a basis for making fundamental analyses of the natural mixing and dispersion processes in a large body of water.

Typically, wind generated currents are an important factor in the near surface dispersion process. However, as wind action is usually unstable, the dispersion patterns which result from the injection of tracer materials are often erratic and heavily skewed thus making the analysis of field data complex. It was evident that large quantities of field data would be required in order to derive statistical parameters and distribution functions descriptive of the material transport and dispersion characteristics of the water body under investigation.

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[1] References are listed alphabetically in the Bibliography, pgs. 109-111.

The difficulties, time and cost involved in collecting large volumes of data behooves consideration of using other alternatives, such as micro-models to facilitate the description and analysis of short-term, near surface, diffusion processes. In the past some of the most valuable interpretative studies of dispersion phenomena have been performed in laboratories under controlled conditions. Thus, it is reasoned that a micro-model which can serve to describe and analyze the short-term dispersion process would be a valuable adjunct to field investigations. The model could reduce substantially the amount of field data necessary for the verification and documentation of dispersive patterns.

Finally, the numerical model approach offers opportunities for the rapid simulation of a wide variety of flow concentrations and dispersion situations by providing insight into the dispersion process and by reducing the amount of field data to be collected. As a consequence, research efforts can be focused on more comprehensive testing, verification and evaluation of dispersive phenomena.

The mathematical solution of the dispersion equation utilizing newer combinations of finite difference procedures and computer technology offers opportunities to undertake dispersive type studies in various flow situations on a more comprehensive basis than a straight field investigation in a given reservoir. Many previously developed analytical techniques have been based on simplifying assumptions which often curtail the range of initial and boundary conditions and exclude the concurrent consideration of other vital factors such as shear flow.

1-2 Background Information

The most easily obtained analytical solution expresses one dimensional convective diffusion for steady uniform flow with a constant diffusion coefficient in an infinite space. Extensions of the one dimensional solution to two and three dimensions are reported by Diachishin [1963] and Glover [1964] and are applicable for steady, uniform flow with constant diffusion coefficients. Taylor [1954] made a one dimensional solution applicable for convective shear flow in pipes by developing an equation which combines the radial dispersive effects of shear flow and the longitudinal turbulent diffusion coefficient into one term, the dispersion coefficient. Using procedures similar to that of Taylor, equations for dispersion coefficients have been developed for other flow conditions, notably Elder [1959] and Fischer [1966] for two dimensional shear flow in open channels and Bowden [1965] for two dimensional shear flow with applications to estuaries and the sea. Two dimensional steady flow problems may be reduced to one dimensional problems by using steady state dispersion coefficients. The user can then employ the one dimensional convective diffusion equation to produce an approximate concentration distribution.

Results obtained by using dispersion coefficients with the one dimensional convective diffusion equation are often adequate when approximations are sufficient in meeting the needs of the user. Concentration distributions based upon dispersion coefficients are not completely accurate when describing most naturally occurring flow conditions. This is because the dispersion coefficients do not include many of the variations which typically occur in moving fluids. The most commonly omitted variations include (a) temporal effects which are negligible only after mixing has spread the material over the channel, (b) longitudinal turbulent diffusion which is important if convective velocities are small, and (c) variations in the turbulent diffusion coefficients which theoretically vary directly with the changes in local shear stresses throughout the moving fluid. The effects of these variations are not always large enough to alter the resulting concentration distribution. But,there exist a large number of practical problems where the inclusion of some of these variations is essential to proper analysis. For these problems numerical solutions offer an opportunity for successful evaluation by a correct, inclusive description of all dispersive phenomena.

Numerical solutions are not without their own unique difficulties. A mathematically correct solution is assured only after a proper analysis is made to confirm stability, convergence and compatibility of the derived solution. The conditions produced by these analyses often impose severe limitations upon problems easily handled by analytical techniques. A partial differential equation can easily be expressed by finite differences, but the finite difference formulation is not always easily solved. For any given class of problems, there often exist several computational algorithms each with its own stability and convergence criteria. Thus, computational experience should indicate which method is the most suitable for a given class of problems in terms of efficiency, accuracy and ease of handling.

1-3 Purpose

The purposes of this study are:

(a) To examine and describe the various computational algorithms for the solution of the two dimensional convective dispersion equation.

(b) To determine the advantages, disadvantages, limitations and general applicability of these numerical algorithms to dispersion problems in which convective shear flow or lateral variations of the mean velocity profile are extant.

(c) To select the most effective algorithm which compositely considers convective shear flow (or lateral variation of the mean velocity profile) as well as lateral and longitudinal diffusion.

1-4 Scope and Methodology

(a) The numerical methods of solution will be examined by the explicit, implicit, and characteristic method.

(b) The computational algorithms will be applied to dispersion problems formulated in a two dimensional space bounded in the transverse direction and semi-infinite in the longitudinal direction. Models will be developed and analysis made of solutions to special problems using each of the three major computational models.

(c) The mathematical models will incorporate numerically the combined dispersive effects of turbulent diffusion and convective shear flow similar in concept to that performed analytically by Taylor [1954].

(d) Using statistical parameters derived from the resulting concentration distributions, the dispersion coefficients will be determined and variations will be noted.

(e) The accuracy and applicability of the numerical dispersion algorithms will be tested and evaluated in the following specific types of flow situations:
   1. Plug flow
   2. Shear flow
   3. Natural open channel flow
   4. Run of the river reservoir flow

(f) Numerical calculations will be programmed for computerized solutions. Notation and conversions utilized will be defined, formats illustrated and computational programming of each of the three methods of flow charted.

Chapter 2

ANALYSIS OF DIFFUSION AND DISPERSION CONCEPTS

2-1 Introduction

Molecular diffusion is the spontaneous intermingling of miscible fluids placed in mutual contact, without the presence of mechanical mixing. However, even in apparently quiescent solutions systems, slight convective currents due to temperature or density gradients within the solution or to residual or undamped mechanical motion, are invariable present to some slight extent.

At high velocities the motion of all fluids becomes turbulent in which case many small eddies, or swirls, cause mixing of parallel streams of the fluid. In such a moving fluid, molecular diffusion does occur but mixing takes place with greater ease and rapidity than with molecular diffusion alone. The transference of material or the mixing of fluids by turbulence has been termed eddy or turbulent diffusion.

Through the years some confusion has existed over the technical usage and interpretation of the words diffusion and dispersion. Much of this confusion can be attributed to the divergent views and differing word use practices of authors in their technical articles. Consequently, many readers have misinterpreted their meanings and have become confused. Recently, attempts have been made to establish a common meaning and word usage among investigators. It has been suggested by Holley [1969] that "diffusion" refer to cases where the transport is primarily associated with time averaged velocity fluctuations and that "dispersion" refer to those cases where the transport is associated with spatially averaged velocity fluctuations. A simpler interpretation can be based on a phenomenological classification.

The three primary phenomenological causes of mixing are (a) molecular diffusion, (b) turbulent diffusion and (c) convective displacement. Whenever a case exists such that the effects of one phenomenon can clearly be separated from the other effects, then the name of the phenomenon should be used in preference to any other description. Molecular diffusion and turbulent diffusion are "diffusion" when no effects of convective dispersion are present. Convective displacement is "dispersion" regardless of any other effects. Turbulent diffusion and convective displacement together result in only further dispersion of the material. In effect, most naturally occurring cases would be dispersion, and only under the most controlled conditions would diffusion exist. Clearly, as Holley suggested, a description of the phenomenon is more informative and should be adhered to when possible, e. g. , longitudinal turbulent diffusion, lateral dispersion. Throughout this report "diffusion" refers to pure molecular and turbulent diffusion and "dispersion" refers to convective displacement and to all combined effects of convective displacement and diffusion.

2-2 Brief Review of Diffusion Laws

Diffusion is a process of concentration equalization, whereby one substance moves through another until a uniform distribution is achieved. On the molecular scale, the driving mechanism is the concentration gradient which is related by the coefficient of molecular diffusion to the quantity of material transported in the direction of negative gradient. This observational relationship is known as Fick's first law of diffusion. For a gradient in the s direction, the rate of mass flux, J, per unit area normal to the s direction may be expressed by

$$J = - D_m \frac{\partial C}{\partial s} \qquad (2.1)$$

where D_m is the coefficient of molecular diffusivity in dimensions of area per unit time, C is the concentration expressed as mass per unit volume, and $\frac{\partial C}{\partial s}$ is the gradient of the concentration in the s direction. Equation (2. 1) expresses one dimensional molecular diffusion across a plane normal to the s direction. Molecular diffusion may be extended to more than one dimension by using vector notation, i. e.,

$$\vec{J} = - D_m \nabla \cdot C \qquad (2.2)$$

As Fick's first law is based on transport across one plane in any given direction, Equations (2. 1) and (2. 2) are hard to use to evaluate unknowns. For example, D_m can only be determined when a steady state condition exists and J and the concentration gradients are measurable. As steady state conditions rarely occur, another expression of diffusion is required.

Again using a one dimensional reference system the principle of conservation of mass is combined with Fick's first law to express net transport of diffusant between two planes normal to the s direction. If a volume element of incompressible fluid bounded by two parallel planes located at s and s+ds is considered, then the change in flux between the two planes is determined by

$$J_s - J_{s+ds} = J_s - \left(J_s + \frac{\partial J_s}{\partial s}\, ds\right)$$

and by substituting Fick's first law for J_s

$$\frac{\partial J_s}{\partial s}\, ds = -\left[\partial\left(D_m \frac{\partial c}{\partial s}\right)/\partial s\right] ds \qquad (2.3)$$

During a time interval the change in flux must be equivalent to the change in concentration within the volume element, i. e.,

$$\frac{\partial c}{\partial t} = \partial\left(D_m \frac{\partial c}{\partial s}\right)/\partial s \qquad (2.4)$$

or in vector notation with constant molecular diffusivity as

$$\frac{\partial c}{\partial t} = D_m\ \nabla^2 \cdot c \qquad (2.5)$$

Thus, diffusion is expressed as a function of the rate of change of the concentration gradient. This expression is known as Fick's second law of diffusion and may be applied to steady or unsteady flows in one or more directions.

2-3 Analysis of the Convective-Diffusion Equation

2-3a Basic Formulation.

The foregoing mathematical expressions for diffusion must be modified by the introduction of convective velocity if a fluid is in motion. Assuming one dimensional flow within a volume element bounded by two parallel planes at s and s+ds, the change in concentration within the volume element is expressed by:

$$\Delta C = \frac{1}{\Delta S}\left[(uC)_s - (uC)_{s+ds}\right]dt \qquad (2.6A)$$

where u is the convecting velocity and C is the diffusant concentration, or in differential equation form, Equation (2. 6A) can be written as

$$\frac{\partial c}{\partial t} = -\frac{\partial (uC)}{\partial S} \qquad (2.6B)$$

The convection can be expressed vectorially and then combined with Equation (2. 5) to express the convective diffusion equation as

$$\frac{\partial c}{\partial t} = D_m \nabla^{2}\cdot C - u\,\nabla\cdot C \qquad (2.7)$$

A detailed development of these relations is found in the work of Dailey and Harleman [1966].

2-3b Reynolds Analogy. In 1874 while studying the transfer of heat from a plate to a convecting fluid, Osborn Reynolds recognized the similarity between the transport processes of molecular diffusion and the diffusive effects of the turbulent motion within the convecting fluid. This assumption of similarity led to the development of some simple, useful equations within the research fields of heat and mass transfer. The equations relate friction factors to coefficients of heat and mass transfer and may be found in such texts as Bennett and Myers [1962]. Since Reynolds' time the principle of the Reynolds analogy has been utilized in application to the turbulent transport processes of momentum, heat and matter. Hinze [1959] showed that an analogy between any two processes is valid if (a) the corresponding differential equations and the initial and boundary conditions are identical for each phenomenon, and (b) the flow field is free from external influences and, also, free of sources and sinks.

2-3c Turbulent Diffusion. Turbulent diffusivity is defined in terms of the mass transport of the diffusant. The momentum transfer as a function of the time averaged velocity fluctuations is expressed by the Reynolds' stresses as

$$-\rho \overline{u_i' u_j'} \qquad (2.8)$$

where ρ is the mass, u' is the instantaneous velocity fluctuation relative to the temporal mean velocity, the subscripts j and i are vector directions normal to each other, and the bar refers to the time average of the product of the instantaneous velocity vectors. A similar analysis may be made with mass transport by turbulent eddy motion with the use of Reynolds analogy. Thus, the turbulent mass flux per unit area is

$$\overline{u_i c'} \qquad (2.9)$$

where c' is the instantaneous fluctuation from the mean concentration and is expressed as mass per unit volume. As all diffusion processes are gradient dependent, then by applying Fick's first law and assuming Reynolds analogy, the turbulent mass flux is related to the concentration gradient by the turbulent diffusion coefficients, i. e.,

$$\overline{u'c'} = -E_i \frac{\partial \overline{C}}{\partial x_i} \qquad (2.10)$$

where E is the turbulent diffusion coefficient and i is the vector direction. For isotropic turbulence E_x, E_y and E_z are equal.

Although the definition of the turbulent diffusion coefficient is widely acknowledged, it is seldom directly applied in diffusion computations for moving fluids. No efficient computational solutions of the diffusion equation exist in which temporal and spatial variations of the coefficient may be included. Before an analytical solution can be utilized, a time averaged coefficient of diffusion must be determined. Consequently, research efforts have concentrated on defining the time averaged coefficients of turbulent diffusivity for steady state conditions.

The turbulent flow counterpart to the convective diffusion equation may be derived by following a procedure similar to that employed in the development of Equation (2.7). Essentially, the equation is derived in an analogous manner and sums the effects of convection, molecular diffusivity and turbulent diffusivity and is stated vectorially as

$$\frac{\partial C}{\partial t} = D_m \nabla^2 \cdot C + \nabla \cdot (E_i \nabla \cdot C) - u_i \nabla \cdot C \qquad (2.11)$$

This equation accounts for all dominant influences upon a conservative substance diffusing through an incompressible fluid. Seldom is the expression employed as stated above. Usually several simplifying assumptions are made to eliminate those phenomena whose effects are negligible in proportion to those of the predominant phenomena.

2-3d Convective Shear Flow. Shear flow refers to a broad class of motion for real fluids. Though nonexistent, a moving, ideal fluid would be frictionless and have no internal shear stresses. Thus, it would move uniformly along a channel with no velocity gradient. A real fluid, however, is not frictionless and develops internal shear stresses. Influences of boundaries and other external forces upon a moving fluid cause friction, and thus, shear stresses develop between the moving fluid elements due to viscosity and turbulent momentum transfer. The variation in magnitude of the shear stresses causes adjacent fluid particles to move along a channel with different velocities and to form a velocity distribution. A flow with a velocity distribution may be regarded as shear flow.

For most moving fluids, convective shear flow is recognized as the greatest contributing phenomena to the dispersion of a material. Tracer material contained in a fluid element is physically displaced or convected a distance $dx = \bar{u}_l(dt)$ during the time period dt where $\bar{u}_l$ is the local temporal mean velocity. Vertically and laterally adjacent fluid elements may be convected at different mean local velocities and would be physically displaced from each other by a distance equal to the local velocity difference multiplied by the time period. This displacement of adjacent fluid elements which contain tracer material is commonly termed convective displacement.

Convective displacement is generally viewed over the cross section of a moving fluid. The mean velocity profile over the cross section provides the measure of the average convective displacement over a unit time period. Figure (2-1b) illustrates the convective displacement of tracer material for a hypothetically surface generated current. When the displacement of tracer material is summed over the cross section, the longitudinal dispersion is obtained as shown in Figure (2-1c). This is the same mechanism which G. I. Taylor [1954] considered when analyzing dispersion in turbulent flow through a pipe. His results show the dominance of shear flow in dispersing material. For turbulent flow in pipes, the effects of convective displacement are two hundred times greater than the effects of longitudinal turbulent diffusion. Whenever turbulent shear flow occurs, the effects of convective displacement are predominant, and these effects are the basis of the dispersion coefficients.

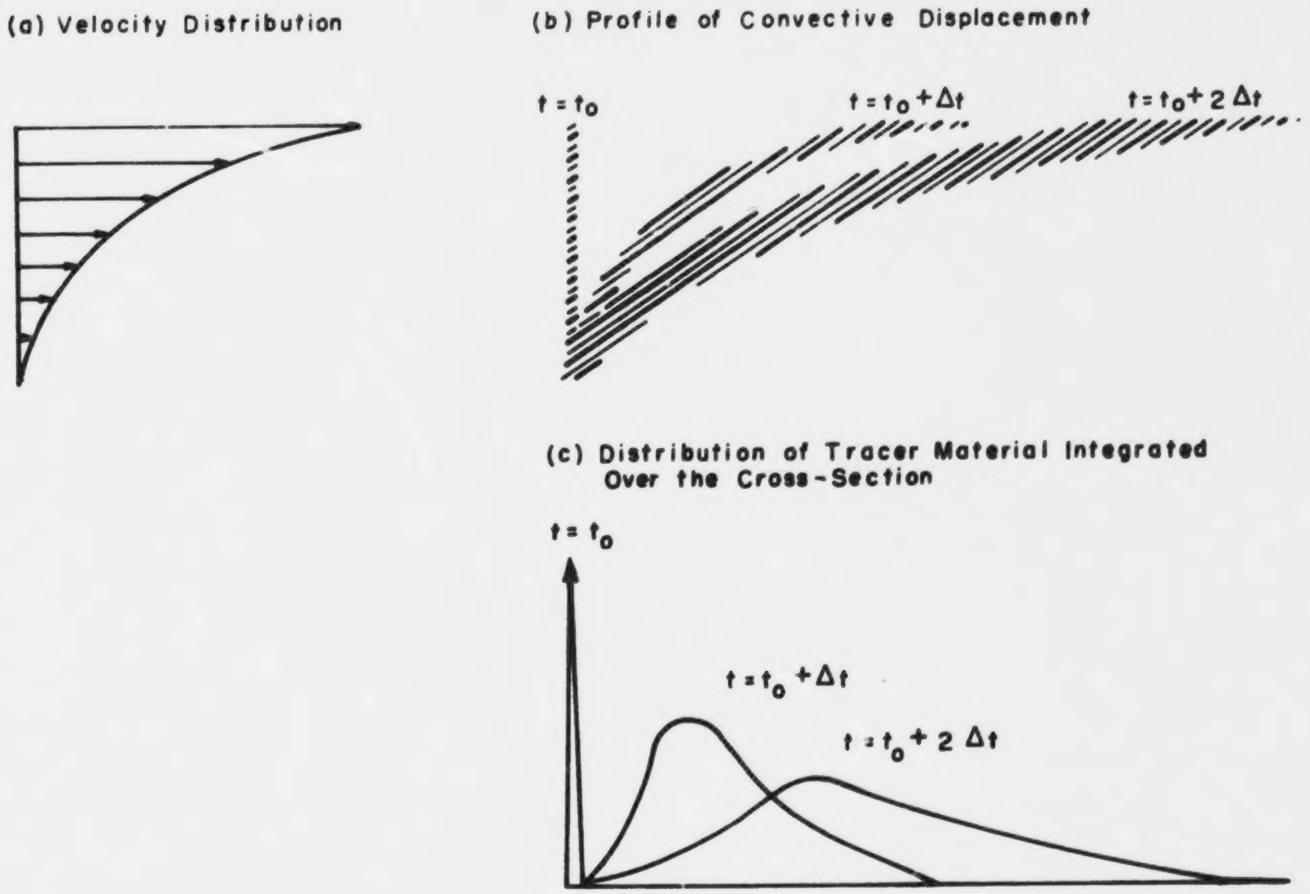
2-4 Formulation of the Two Dimensional Convective Dispersion

As stated in Chapter 1, this study is concerned with the two dimensional convective dispersion equation which includes turbulent diffusion and convective displacement. Equation (2.11) was developed as the convective dispersion equation. When the velocity varies and convective displacement occurs, Equation (2.11) becomes the convective dispersion equation,

$$\frac{\partial C}{\partial t} = D_m \nabla^{2} \cdot C + \nabla \cdot (E_i \nabla \cdot C) - u_i \nabla \cdot C \qquad (2.11)$$

To limit Equation (2.11) to two dimensions, the following assumptions are made.

(a) The effects of molecular diffusion are so small when turbulent flow exists that molecular diffusion may be



(a) Velocity Distribution

(b) Profile of Convective Displacement

(c) Distribution of Tracer Material Integrated Over the Cross-Section

FIGURE 2-1 CONVECTIVE DISPLACEMENT OF TRACER MATERIAL FOR A HYPOTHETICAL SURFACE GENERATED CURRENT

neglected.

(b) The phenomenon is two dimensional in nature, i. e., the dispersive effects are viewed over a plane with the effects in the direction normal to the plane being uniform. Let the directional vector x correspond to the longitudinal direction, and let y be normal to x. Note that y may refer to either the lateral or vertical direction.

(c) The convection is unidirectional in the x direction, i. e., the mean velocity is zero in the y direction.

Applying the above assumptions to Equation (2. 11), the two dimensional convective dispersion equation is

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(E_x \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(E_y \frac{\partial c}{\partial y}\right) - \bar{u}_L \frac{\partial c}{\partial x} \qquad (2.12)$$

where $\bar{u}$ is the mean local velocity in the x direction. When applying this equation to a grid in x, y and t space, the values of the variables may be applied as constants at any point (x,y and t) on the grid, see Richtmyer [1957]. Thus, for the variables of E_x, E_y and u varying with x, y and t, Equation (2. 12) becomes

$$\frac{\partial c}{\partial t} = E_x (x, y, t) \frac{\partial^2 c}{\partial x^2} + E_y (x, y, t) \frac{\partial^2 c}{\partial y^2} - u(x, y, t) \frac{\partial c}{\partial x} \qquad (2.13)$$

For the purposes of this study, the following simplifying assumptions are made: (a) E_x and E_y remain constant, and (b) u varies only in the direction normal to x. Equation (2. 13) becomes

$$\frac{\partial c}{\partial t} = E_x \frac{\partial^2 c}{\partial x^2} + E_y \frac{\partial^2 c}{\partial y^2} - u(y) \frac{\partial c}{\partial x} \qquad (2.14)$$

and is the two dimensional convective dispersion equation which is studied in this investigation. Thus, the equation to be dealt with contains two dimensional turbulent diffusion with uniform coefficients and convective displacement.

Chapter 3

MODELS FOR SOLUTIONS OF CONVECTIVE DIFFUSION AND DISPERSION PROBLEMS

3-1 Introduction

Solutions of the convective dispersion problem have been presented in a variety of ways. There have been both solutions by exact mathematical analysis and approximations of the physical process by numerical modeling. Each solution, whether obtained by mathematical analysis or numerical modeling of the physical process, can be used to predict the distribution of material in a moving fluid provided that the initial and boundary conditions are satisfied. As stated previously, this study is concerned with dispersion problems represented by Equation (2. 14) and formulated in a two dimensional space bounded in the transverse direction and semi-infinite in the longitudinal direction.

With the absence of the convective terms, the two dimensional diffusion equation is classified as a parabolic partial differential equation and is expressed as

$$\frac{\partial c}{\partial t} = D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2} \qquad (3.1)$$

Equation (3. 1) is commonly known as the heat flow equation, the diffusion equation or the mass transfer equation depending upon which phenomenon is represented. D_x and D_y are the diffusion coefficients for the phenomenon. For turbulent diffusion the coefficients become E_x and E_y and are known as the coefficients of turbulent diffusion. Equation (3. 1) then becomes the two dimensional turbulent diffusion equation, i. e.,

$$\frac{\partial c}{\partial t} = E_x \frac{\partial^2 c}{\partial x^2} + E_y \frac{\partial^2 c}{\partial y^2} \qquad (3.2)$$

Whenever unidirectional convection is present, the equation remains, basically, a parabolic partial differential equation, and is expressed as

$$\frac{\partial c}{\partial t} = E_x \frac{\partial^2 c}{\partial x^2} + E_y \frac{\partial^2 c}{\partial y^2} - u \frac{\partial c}{\partial x} \qquad (3.3)$$

To be consistent with the definitions presented in Chapter 2, Equation (3. 3) is known as the convective diffusion equation whenever a velocity is present but its lateral variations have no effect upon the mixing of the material, e. g., plug flow. Equation (3. 3) is known as the convective dispersion equation whenever a velocity is present and its lateral variations contribute to the mixing of the material, e. g., shear flow. An efficient numerical solution to Equation (3. 3) is the goal of this study. Previous work on this problem is presented beginning with numerical models approximating physical processes.

3-2 Numerical Models Approximating the Physical Process

Whenever mathematical solutions to a problem are nonexistent or difficult to obtain, engineers often construct approximate numerical models of the physical process. An excellent example is the model constructed by Fischer [1966a] in his work on natural streams. Fischer was concerned with the dispersion of material injected into the stream from an instantaneous batch type source and uniformly mixed over the cross section.

To model the physical process, Fischer divided the stream's cross section into ten or less stream tubes. Each tube being characterized by a velocity dependent upon the position of the stream tube. For a time step Δt the mass within each tube moves a distance

$$\Delta x = u_i \Delta t \tag{3.4}$$

where u_i is the velocity within the tube. Within each time step the following two events occur: (a) the concentration distribution within each stream tube moves upstream or downstream a distance dependent on the velocity of the tube; (b) at grid points within the cross section the concentration is transferred to adjacent tubes in a proportion consistent with dispersion coefficients. This process is repeated for each time step. Fischer reports a close correlation between the results of this modeling procedure and concentration distributions collected in laboratory experiments.

Fischer's model couples the effects of lateral turbulent diffusion and convective displacement. The effects of longitudinal turbulent diffusion are neglected. The graphical presentation of Fischer's experimental and numerical results show (a) a marked frontal effect for the leading edge of the concentration plume and (b) an earlier and higher peaking for the experimental results when compared with the numerical results. Nevertheless, Fischer has shown that good predictive results can be obtained by proper modeling of the physical processes and without rigid mathematical analysis.

Another example of the realistic application of the numerical model is indicated in Fischer's [1968] recent report. Fischer applies specific analytical methods developed in his earlier works for predicting and checking the accuracy of dispersion coefficients in natural streams. Specifically, Fischer tested his method by comparison with actual field data obtained by other experimenters during ten tests in six natural streams.

Fischer states that a theoretically exact method for calculating a dispersion coefficient from concentration versus time curves obtained at two stations on a stream is:

$$D = \frac{1}{2}\,\bar{u}^2 \frac{\sigma_{t_2}^2 - \sigma_{t_1}^2}{\bar{t}_2 - \bar{t}_1}$$

in which $\sigma_{t_1}^2$ and $\sigma_{t_2}^2$ are the variances of the concentration time curves at the upstream and downstream stations, respectively, and $\bar{t}_1$ and $\bar{t}_2$ are mean times of passage of the tracer cloud past each station. The restriction placed on use of this equation is that both stations must be downstream at such a distance so that during passage of the tracer cloud its behavior is approximated by the one dimensional dispersion equation in which the local velocity is replaced by a mean value.

In other words, this form of dispersion equation should not be applied to a dispersing tracer cloud until after the initial or convective period has transpired. Within the convective period the tracer distribution is sharply skewed, the concentration rises steeply at the downstream end and trails off slowly upstream. This obviates the need for the special conditions regarding the location of the two stations. However, it is evident that this criteria precludes consideration of dispersion on a micro-model basis.

In the Fischer tests, the accuracy of the computed dispersion coefficient is checked by an integration procedure based on dispersion theory. The upstream observed concentration curve is used as the initial tracer distribution and a concentration time curve for the downstream station is predicted by the one dimensional dispersion model cited above. The predicted and observed downstream station curves are compared. If the values are not reasonably close, a new dispersion coefficient is selected and the calculation is repeated until the best possible comparison is obtained. Fischer terms this procedure "the routing procedure," due to its similarity to flood routing.

Fischer concluded that:

(a) Agreement between predicted and observed curves was usually good for experiments in which dimensionless time[2], $t' > 10$ at the upstream station. For lower values of dimensionless time errors occur due to tracer cloud not performing according to the one dimensional dispersion equation and conversion from concentration-time curves is less accurate at low time values.

(b) Procedure was accurate whenever $t' > 4$ at the upstream station and > 6 at the downstream station.

(c) From the viewpoint of wastewater engineering, - "the usual objective of dispersion theory is to allow the engineer, knowing the distribution of a pollutant at some upstream station, to predict the pattern at a downstream station, in particular the expected duration of cloud passage and peak concentration. A dispersion coefficient obtained by any method is of no value unless it predicts correctly these quantitics."

The feasibility and versatility of the numerical model approach is demonstrated further by the recent work of Harleman, et al [1968] who developed an implicit solution to the one dimensional mass transfer equation which describes the advective motion (including the tidal and fresh water flows) and the longitudinal dispersion for a one dimensional variable area estuary of arbitrary geometry. The results of the model were then compared with field measurements of dye dispersion performed by other investigators in the fresh water tidal portion of the Potomac estuary.

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[2] Defined as $t' = \frac{t}{T}$ in which T = the Lagrangian time scale: $T = 0.30 \frac{l^2}{ru*}$

l = characteristic length of channel
r = hydraulic radius
u* = shear velocity
t = time

Harleman, et al, used an implicit formulation because of the stringency of the stability requirements on an explicit solution for low dispersion coefficients. This study showed that dispersion coefficients and concentration distributions could be predicted by numerical methods. However, this work also assumes that the convective period has transpired and that the process can be described by the one dimensional dispersion equation utilizing a mean velocity over any cross-section.

3-3 Analytical Solutions

Analytical solutions of the convective diffusion equation have their roots in operational and transformational mathematics of parabolic partial differential equations. The mathematical derivation of the solution will not be presented, only the resulting solution. The equation for one dimensional turbulent diffusion of a slug of injected material is

$$\frac{\partial C}{\partial t} = E_x \frac{\partial^2 C}{\partial x^2} \qquad (3.5)$$

where C is the concentration in mass per volume, t is time, x is distance, and E_x is the coefficient of turbulent diffusion. The solution of Equation (3. 5) for boundaries of infinite extent is

$$C = \frac{C_o}{\sqrt{4\pi E_x t}} \exp -(x^2/4 E_x t) \qquad (3.6)$$

where C_o is the initial concentration of the slug in mass per unit volume. Thus, C denotes the concentration at point x and time t.

For the one dimensional convective diffusion equation,

$$\frac{\partial c}{\partial t} = E_x \frac{\partial^2 c}{\partial x^2} - \bar{u}\frac{\partial c}{\partial x} \qquad (3.7)$$

with $\bar{u}$ being the mean convection, the solution is

$$C = \frac{C_o}{\sqrt{4\pi E_x t}} \exp\left[-(x-\bar{u}t)^2/4E_x t\right] \qquad (3.8)$$

Equation (3. 8)[3] is based upon the solution of Equation (3. 5) after making a coordinate change in Equation (3. 7). The solution of Equation (3. 5) is the most easily attained solution and is the solution upon which most extensions are based.

---

[3] The equation:

$$C = \frac{C_o}{\sqrt{4\pi E_x t}} \exp\left[-(x-\bar{u}t)^2/4E_x t\right]$$

can be re-written as:

$$\frac{C}{C_o} = \frac{1}{\sqrt{2E_x t}\,\sqrt{2\pi}} \cdot \exp\left[-\left(\frac{1}{2}\right)\left(\frac{x-\bar{u}t}{\sqrt{2E_x t}}\right)^2\right]$$

In the above form, its conformance to a normal distribution equation is readily apparent. For a normal distribution the equation is:

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right]$$

where: σ = standard deviation, and
μ = mean

Thus, $\frac{C}{C_o}$ follows a normal curve along the x direction for which the standard deviation, $\sigma = \sqrt{2E_x t}$ and, the mean, $\mu = \bar{u}t$.

Diachinshin [1963] and Glover [1964] present solutions to two and three dimensional representations. For the equation of two dimensional convective diffusion

$$\frac{\partial c}{\partial t} = E_x \frac{\partial^2 c}{\partial x^2} + E_y \frac{\partial^2 c}{\partial y^2} - \bar{u}\frac{\partial c}{\partial x} - \bar{v}\frac{\partial c}{\partial y} \qquad (3.9)$$

where $\bar{v}$ is the mean velocity in the y direction and E_y is the coefficient of turbulent diffusion in the y direction, the solution is

$$C = \frac{C_o}{2\pi}\,\frac{\exp-[(x-\bar{u}t)^2/4E_x t]}{\sqrt{2E_x t}} \cdot \frac{\exp[(y-\bar{v}t)^2/4E_y t]}{\sqrt{2E_y t}} \qquad (3.10)$$

Thus, for the two dimensional diffusion equation with convection occurring only in the x direction, the solution is

$$C = \frac{C_o}{2}\,\frac{\exp-[(x-\bar{u}t)^2/4E_x t]}{\sqrt{2E_x t}} \cdot \frac{\exp-(y^2/4E_y t)}{\sqrt{2E_x t}} \qquad (3.11)$$

Both Diachinshin and Glover extend this analysis to include the third dimension, z.

The above equations do not describe the concentration distributions which occur in most moving fluids because only the mean velocity of the moving fluid mass is considered and the dispersive nature of shear flow is neglected. That is, the convective diffusion problem is solved instead of the more common problem of convective dispersion.

Taylor [1954] developed a method for solving the convective dispersion problem. Using the "universal" velocity distribution for turbulent flow in a pipe, Taylor integrated the displacements of the velocity distribution over the cross section, related the sum of the integration to the rate of transfer across a section, and then computed a coefficient of dispersion to be

$$E'_T = 10.06\ Ru^* \tag{3.12}$$

where R is the radius of the pipe, u* is the shear velocity, and E'_T is a coefficient of dispersion. Taylor then evaluated longitudinal turbulent diffusion in terms of R and u*, thus, the mean coefficient of longitudinal turbulent diffusion, E'_x, is

$$E'_x = 0.052\ Ru^* \tag{3.13}$$

Note that the dispersive effects of longitudinal shear flow are 200 times greater than the effects of longitudinal turbulent diffusion. Taylor assumed that these effects are additive; thus, his well known dispersion coefficient for turbulent flow in a pipe is

$$E_T = (10.06 + 0.05)\ Ru^* = 10.1\ Ru^* \tag{3.14}$$

where E_T is the dispersion coefficient representing the total effects of dispersion.

Elder [1959] followed Taylor's analysis and developed a dispersion coefficient for turbulent shear flow in an open channel of infinite width, as

$$E_T = 5.93\ hu^* \tag{3.15}$$

where h is the depth and u* is the shear velocity. Fischer [1966a], investigating dispersion in natural streams, found the lateral velocity distribution to be the controlling velocity profile instead of the vertical velocity profile used by Elder. Fischer presents an inclusive definition of the dispersion coefficient in terms of functional relationships for the velocity distribution, cross sectional area and turbulent diffusion coefficients. A thorough explanation may be found in Fischer's 1966a and 1967 publications.

Bowden [1965], following an analysis similar to that of Taylor and Elder, developed a dispersion coefficient for application in the sea. Being general for application to any velocity distribution as is Fischer's, the coefficient is determined from several functional statements. An explanation of the functional statements and the dispersion coefficient and how they are applied appears in his publication.

The principal advantage of developing a total dispersion coefficient is that this coefficient may be substituted for the diffusion coefficient in the solution equation of one dimensional convective diffusion, Equation (3. 8). The use of the total dispersion coefficient and the mean velocity in Equation (3. 8) produces a good approximation of the resulting distribution of convective dispersion. Thus, in effect, a phenomenon of two spatial dimensions is approximated in a one dimensional model. As previously shown, Equation (3. 11) describes the resulting distribution of two dimensional diffusion with one dimensional convection. As a dispersion coefficient in Equation (3. 8) describes convective dispersion, and as Equation (3. 11) describes two dimensional convective diffusion, then for most commonly occurring problems of mixing in moving fluids a better approximation is gained by substituting a dispersion coefficient in Equation (3. 8) rather than by using the two dimensional analytical solution, Equation (3. 11).

3-4 Numerical Methods

3-4a Basic Considerations.

Numerical procedures for solving partial differential equations are based on approximations of partial derivatives by finite differences. Finite difference substitutes for the partial derivatives can be derived by applying finite difference calculus to a function, Kunz [1957], or by a Taylor's series expansion of a function, Smith [1965], when the derivatives of the function are single valued, finite, and continuous. Both procedures yield the same approximations and the same error statement.

Consider one spatial dimension represented by the s axis and a dependent variable ϕ . Represent the s axis by I points which equally divide the s axis into I-1 intervals of Δs. First order partial derivatives may then be determined by

$$\frac{\partial \phi}{\partial s} = \frac{\phi_{i+1} - \phi_i}{\Delta s} + O(\Delta s) \qquad (3.16)$$

where $O(\Delta s)$ indicates an error proportional to the magnitude of Δs. Equation (3. 16) without the error term is referred to as the forward difference approximation because the direction is positive from point i. Likewise, the backward difference approximation to the first order partial differential is

$$\frac{\partial \phi}{\partial S} = \frac{\phi_i - \phi_{i-1}}{\Delta S} \qquad (3.17)$$

Sometimes the first order partial differential must be evaluated over two intervals; thus,

$$\frac{\partial \phi}{\partial S} = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta S} + O(\overline{\Delta S}^2) \qquad (3.18)$$

and without the error term Equation (3. 18) is referred to as the central difference approximation.

From the same physically assumed conditions, both derivation procedures yield the expression of the second order partial derivatives to be

$$\frac{\partial^2 \phi}{\partial S^2} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{(\Delta S)^2} + O(\overline{\Delta S}^2) \qquad (3.19)$$

To facilitate expression, Equation (3. 19) is expressed in mathematical shorthand as

$$\Delta_s^2(\phi_i) = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{(\Delta S)^2} \qquad (3.20)$$

Crank and Nicolson [1947] in solving the time dependent heat flow equation, averaged the second order partial derivative over two time intervals. Thus, for time values k and k + 1 the approximation to the second order partial derivative is

$$\frac{\partial^2 \phi}{\partial s^2} = \frac{1}{2}\; \frac{\phi_{i+1,k} - 2\phi_{i,k} + \phi_{i-1,k}}{(\Delta s)^2} + \frac{\phi_{i+1,k+1} - 2\phi_{i,k+1} + \phi_{i-1,k+1}}{(\Delta s)^2} \qquad (3.21)$$

or

$$\frac{\partial^2 \phi}{\partial s^2} = \frac{1}{2}\left[\Delta_s^2(\phi_k) + \Delta_s^2(\phi_{k+1})\right] \qquad (3.22)$$

The Crank-Nicolson approximation is a more accurate approximation than Equation (3. 19) because it reduces the order of magnitude of the error in the time approximation from $O(\Delta t)$ to $O(\Delta t^2)$. Numerical procedures depend upon the proper substitution of the above approximations for the partial differentials of an equation.

Whenever the finite difference approximation yields a stable solution that converges to the solution of the differential equation, the finite difference scheme is said to be compatible with the partial differential equation. Compatibility is determined by evaluating the difference between the differential equation and the difference equation. When this difference becomes increasingly smaller as the grid increments tend to zero, the difference equation is compatible with the differential equation, and proper substitution of finite differences has been made.

The conditions within the finite difference scheme must be such that the solution using the finite difference scheme approximates the exact solution of the differential equation. Let S represent the exact solution of the differential equation with x and t being independent variables, and let s represent the solution using the finite difference scheme. When s approaches S as Δx and Δt approach zero, the finite difference scheme is said to be convergent. Convergence is generally proved by evaluating the conditions under which the maximum possible differences between the solutions tend to zero. Further comments on convergence and illustrations on procedures for evaluating convergence exist in Smith [1965], Richtmyer [1957], Forsythe and Wasow [1960], and other books on numerical analysis.

Conditions within the finite difference representation must also be such that successive computations are stable. Errors occur constantly in numerical procedures due to round off or truncation of sets of infinite numbers of digits into finite numbers of digits. Whenever an error grows in magnitude with successive computations, the finite difference scheme is said to be unstable. If an error decreases in magnitude with successive computations, the finite difference scheme is said to be stable. Stability conditions can be computed either by matrix methods or by the Fourier series method. Further commentary on stability may be found in the previously mentioned references.

A correct solution by numerical methods is assured by an analysis of convergence, compatibility and stability and by an adherence to the conditions thusly imposed. The literature of numerical analysis contains many different numerical schemes along with analyses of stability, convergence and compatibility. Thus, whenever using previously investigated numerical schemes, stability and convergence conditions are generally available. Whenever using a newly developed numerical scheme, proper attention should be given to stability, convergence, and compatibility.

The convective diffusion equation has been solved by several of the computational schemes available for the solutions of parabolic partial differential equations. Primarily, the methods used are the explicit scheme and the implicit scheme using Crank-Nicolson approximations. Recently, a method of solving the convective diffusion equation by integrating along characteristic lines has been introduced. The following is a presentation of these three numerical methods and their limiting conditions.

3-4b Explicit Solution. The explicit method is illustrated by substituting the finite approximations of Equations (3. 16) and (3. 19) into the general one dimensional diffusion equation of

$$\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial x^2} \qquad (3.23)$$

Letting i represent the incremental point in the x direction and k represent the incremental point in the t direction, the substitution yields

$$\frac{C_{i,k+1} - C_{i,k}}{\Delta t} = \frac{C_{i+1,k} - 2C_{i,k} + C_{i-1,k}}{(\Delta x)^2} \qquad (3.24)$$

The terms can be rearranged to produce

$$C_{i,k+1} = \left(1 - 2\frac{\Delta t}{\Delta x^2}\right)C_{i,k} + \left(\frac{\Delta t}{\Delta x^2}\right)\left(C_{i+1,k} + C_{i-1,k}\right) \qquad (3.25)$$

Thus, the value of $C_{i,k+1}$, the only unknown, is computed explicitly in terms of the values of C at the previous time increment k. To initiate computations, an evaluation of C_i at k=1 and the boundary conditions for all values of k must be known. With the above requirement this class of parabolic partial differential equations is demonstrated to be properly defined initial value problems.

For the two dimensional convective diffusion equation, consider a three dimensional space with the independent variables of x, y and t. Divide the x axis by I points into (I-1) equal increments of Δx ; divide the y axis by J points into (J-1) equal increments of Δy; and divide the t axis by K points into (K-1) equal increments of Δt. The concentration at point $x=i\Delta x$, $y=j\Delta y$ and $t=k\Delta t$ is hereafter referenced as $C_{i,j,k}$.

For the two dimensional convective diffusion equation

$$\frac{\partial c}{\partial t} = E_x \frac{\partial^2 c}{\partial x^2} + E_y \frac{\partial^2 c}{\partial y^2} - u\frac{\partial c}{\partial x} \qquad (3.3)$$

the substitution of the finite difference approximations yields

$$\frac{C_{i,j,k+1} - C_{i,j,k}}{\Delta t} = \frac{E_x}{\Delta x^2}\left(C_{i+1,j,k} - 2C_{i,j,k} + C_{i-1,j,k}\right)$$
$$+ \frac{E_y}{\Delta y^2}\left(C_{i,j+1,k} - 2C_{i,j,k} + C_{i,j-1,k}\right)$$

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$$- \frac{u}{2\Delta x} \left(C_{i+1,j,k} - C_{i-1,j,k} \right) \quad (3.26)$$

The convective term is approximated over a two step interval to maintain the same magnitude of error, $(\Delta X)^2$, as the second order terms and to insure stability, Richtmyer [1957]. When Equation (3.26) is solved for the only unknown $C_{i,j,k+1}$, the relationship becomes

$$\begin{aligned} C_{i,j,k+1} = {} & C_{i,j,k} \left(1 - 2 \epsilon_x \frac{\Delta t}{\Delta x^2} - 2 \epsilon_y \frac{\Delta t}{\Delta y^2}\right) \\ & + C_{i+1,j,k} \left(\epsilon_x \frac{\Delta t}{\Delta x^2} - u \frac{\Delta t}{2\Delta x}\right) \\ & + C_{i-1,j,k} \left(\epsilon_x \frac{\Delta t}{\Delta x^2} + u \frac{\Delta t}{2\Delta x}\right) \\ & + C_{i,j+1,k} + C_{i,j-1,k}) \, \epsilon_y \frac{\Delta t}{\Delta y^2}) \end{aligned} \quad (3.27)$$

The explicit molecule corresponding to this equation is shown in Figure (3.1).

The stability of the one dimensional diffusion equation, Equation (3.24), has been shown by Richtmyer [1957] and others to depend upon a value of $r < \frac{1}{2}$ where

$$r = \frac{\Delta t}{\Delta x^2} \quad (3.28)$$

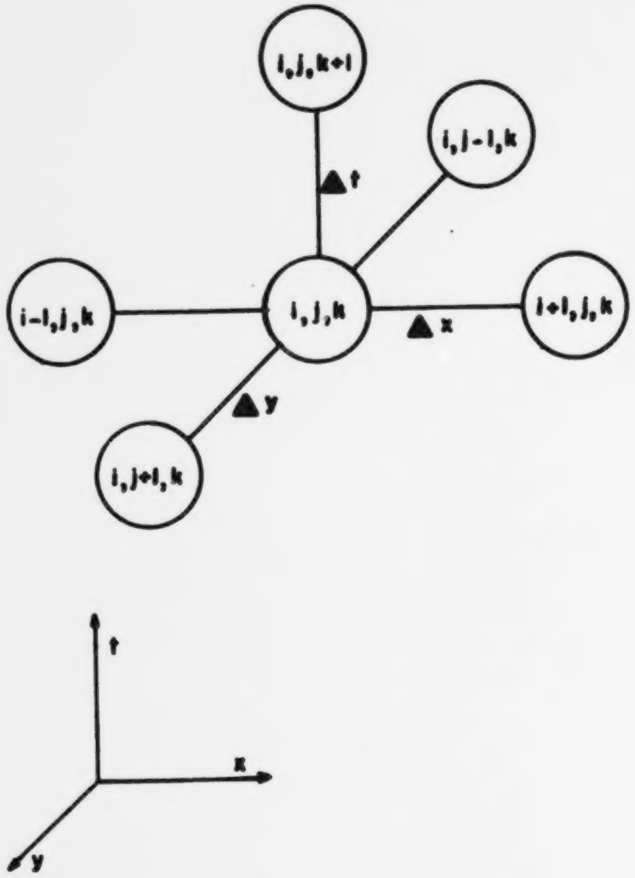

FIGURE 3-1 EXPLICIT MOLECULE FOR TWO DIMENSIONAL CONVECTIVE DISPERSION EQUATION

Kent [1960] points out that in meeting this condition, all of the values by which any C is multiplied are positive, i. e., from Equation (3. 25)

$$1 - 2\frac{\Delta t}{\Delta x^2} > 0 \quad \text{and} \quad \frac{\Delta t}{\Delta x^2} > 0 \qquad (3.29)$$

Whenever an equation is being solved by explicit numerical methods, it can be demonstrated that the conditions of stability are always met whenever the multiplying factor of the dependent variable is positive. Thus, for Equation (3. 27), the conditions of stability are

$$1 - 2E_x\frac{\Delta t}{\Delta x^2} - 2E_y\frac{\Delta t}{\Delta y^2} > 0 \qquad (3.30)$$

and

$$E_x\frac{\Delta t}{\Delta x^2} - u\frac{\Delta t}{2\Delta x} > 0 \qquad (3.31)$$

Equation (3. 31) can be evaluated to show that

$$\Delta x < \frac{2E_x}{u} \qquad (3.32)$$

and Equation (3. 30) can be evaluated to show that

$$\Delta t < \frac{\overline{\Delta x}^2 \cdot \overline{\Delta y}^2}{2(E_x\Delta y^2 + E_y\overline{\Delta x}^2)} \qquad (3.33)$$

Thus, maximum values of the step sizes Δx and Δt can be evaluated. When using turbulent diffusion coefficients which are typically smaller than unity, the value of Δx is less than can be practically used to program a realistic problem on a digital computer. It is this limitation that has discouraged the use of explicit methods to solve most two dimensional convective diffusion problems. Simply stated, enough computer storage does not exist to fit a practical problem on even a large digital computer when the above limitations are applicable.

3-4c Implicit Solution. The implicit method is illustrated by substituting the Crank-Nicolson approximation Equation (3. 21) into the general one dimensional diffusion equation, Equation (3. 23). This substitution yields

$$\frac{C_{i,k+1} - C_{i,k}}{\Delta t} = \frac{1}{2} \quad \frac{C_{i+1,k} - 2C_{i,k} + C_{i-1,k}}{\Delta x^2}$$

$$+ \quad \frac{C_{i+1,k+1} - 2C_{i,k+1} + C_{i-1,k+1}}{\Delta x^2} \qquad (3.34)$$

which is rearranged as

$$\left[\frac{-\Delta t}{2(\Delta x)^2}\right] C_{i-1,k+1} + \left[1 + \frac{\Delta t}{\Delta x^2}\right] C_{i,k+1} + \left[\frac{-\Delta t}{2(\Delta x)^2}\right] C_{i+1,k+1}$$

$$= \left[1 - \frac{\Delta t}{(\Delta x)^2}\right] C_{i,k} + \left[\frac{\Delta t}{2(\Delta x)^2}\right]\left[C_{i-1,k} + C_{i+1,k}\right] \qquad (3.35)$$

In the above equation, three values of C at k+1 are unknown and are expressed in terms of the three known values. The values of C at time step k+1 are said to be expressed implicitly in terms of the known values of C at time step k. This equation is only solved by developing a set of equations for every point i=1 to I. This set of equations can be solved simultaneously with relative ease.

For the two dimensional convective diffusion equation assume the same physical conditions as existed in the presentation of the explicit method. Substituting the first order forward difference approximation, the Crank-Nicolson second order finite difference approximation and the Crank-Nicolson approximation for convection into the two dimensional convective diffusion equation, Equation (3. 3), becomes

$$\begin{aligned}
\frac{C_{i,j,k+1} - C_{i,j,k}}{\Delta t} = {} & \frac{E_x}{2}\left[\frac{C_{i-1,j,k} - 2C_{i,j,k} + C_{i+1,j,k}}{(\Delta x)^2}\right. \\
& \left. + \frac{C_{i-1,j,k+1} - 2C_{i,j,k+1} + C_{i+1,j,k+1}}{(\Delta x)^2}\right] \\
& + \frac{E_y}{2}\left[\frac{C_{i,j-1,k} - 2C_{i,j,k} + C_{i,j+1,k}}{(\Delta y)^2}\right. \\
& \left. + \frac{C_{i,j-1,k+1} - 2C_{i,j,k+1} + C_{i,j+1,k+1}}{(\Delta y)^2}\right] \\
& + \frac{u}{2}\left[\frac{C_{i+1,j,k} - C_{i-1,j,k}}{2\Delta x}\right. \\
& \left. + \frac{C_{i+1,j,k+1} - C_{i-1,j,k+1}}{2\Delta x}\right] \qquad (3.36)
\end{aligned}$$

Equating the unknown values of C to the known values yields

$$
\begin{aligned}
C_{i,j,k+1}\left[-1-\frac{E_x\Delta t}{\Delta x^2}-\frac{E_y\Delta t}{\Delta y^2}\right] &+ C_{i+1,j,k+1}\left[\frac{E_x\Delta t}{2\Delta x^2}-\frac{u\Delta t}{4\Delta x}\right] \\
&+ C_{i-1,j,k+1}\left[\frac{E_x\Delta t}{2\Delta x^2}+\frac{u\Delta t}{4\Delta x}\right] + \left[C_{i,j+1,k+1}\right. \\
&\left.+ C_{i,j-1,k+1}\right]\left[\frac{E_x\Delta t}{2\Delta y^2}\right] = C_{i,j,k}\left[\frac{E_x\Delta t}{\Delta x^2}+\frac{E_y\Delta t}{\Delta y^2}-1\right] \\
&+ C_{i+1,j,k}\left[\frac{u\Delta t}{4\Delta x}-\frac{E_x\Delta t}{2\Delta x^2}\right] + C_{i-1,j,k}\left[-\frac{u\Delta t}{4\Delta x}-\frac{E_x\Delta t}{2\Delta x^2}\right] \\
&+ \left[C_{i,j+1,k}+C_{i,j-1,k}\right]\left[-\frac{E_y\Delta t}{2\Delta y^2}\right]
\end{aligned}
\tag{3.37}
$$

The above equation expresses five unknown values of C at k+1 in terms of five known values of C at k. Three unknown values are on the x axis, and three unknown values are on the y axis. The implicit molecule is shown in Figure (3. 2).

Equation (3. 37) cannot be solved directly but must be solved simultaneously with equations written for each I and J point at time k. The solution of this series of equations is solved by iterative matrix methods based upon procedures developed by Peaceman and Rachford [1955]. These methods are broadly classified as alternating direction implicit procedures (ADIP) and are thoroughly discussed by Varga [1962] and Douglas [1961]. Douglas [1961] presents an alternating

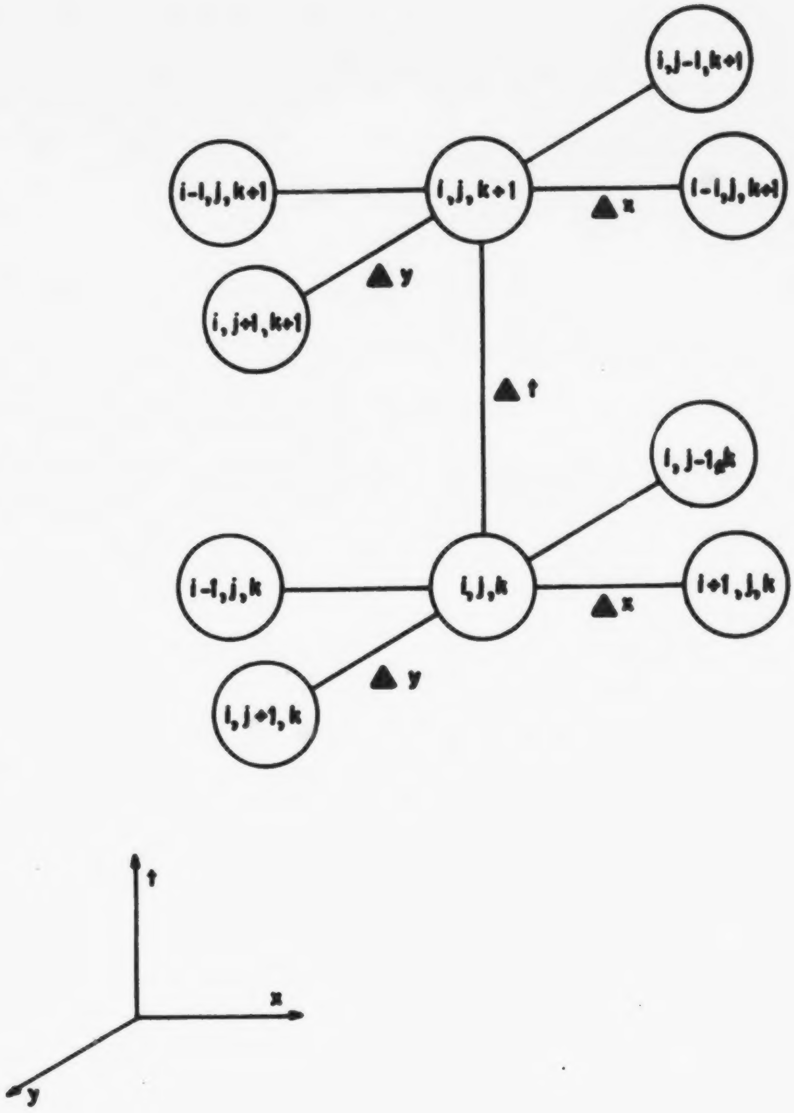

FIGURE 3-2 IMPLICIT MOLECULE FOR TWO DIMENSIONAL CONVECTIVE DISPERSION EQUATION

direction modification to the Crank-Nicolson method. For the solution of the two dimensional convective diffusion equation, first approximate the x-derivative terms by the Crank-Nicolson method. As only the x-derivative terms are approximated and an incomplete solution is attained, the values of C at k+l are expressed as C^*_{k+1} to denote an approximation. The values of C^*_{k+1} can be found from

$$\frac{C^*_{i,j,k+1} + C_{i,j,k}}{\Delta t} = \frac{1}{2}\Delta_x^2\left(C^*_{i,j,k+1} + C_{i,j,k}\right) + \Delta_y^2 C_{i,j,k}$$

$$-\frac{u}{2}\left[\frac{C^*_{i+1,j,k+1} - C^*_{i-1,j,k+1}}{2\Delta x} + \frac{C_{i+1,j,k} - C_{i-1,j,k}}{2\Delta x}\right] \qquad (3.38)$$

Then by using the approximations, C^*_{k+1}, the values of the complete solution, C_{k+1}, can be found by including the Crank-Nicolson approximation to the y derivative term, i. e.,

$$\frac{C_{i,j,k+1} + C_{i,j,k}}{\Delta t} = \frac{1}{2}\Delta_x^2\left(C^*_{i,j,k+1} + C_{i,j,k}\right)$$

$$+ \frac{1}{2}\Delta_y^2\left(C_{i,j,k+1} + C_{i,j,k}\right)$$

$$-\frac{u}{2}\left[\frac{C^*_{i+1,j,k+1} - C^*_{i-1,j,k+1}}{2\Delta x} - \frac{C_{i+1,j,k} - C_{i-1,j,k}}{2\Delta x}\right] \qquad (3.39)$$

In both of the above equations, there are only three unknowns to be found. Writing Equation (3. 38) for all of the x points along a y axis, the values of $C^*_{j,k+1}$ can be determined by simultaneous solution of the series. These values are then used in Equation (3. 39) to establish a more correct value at time k+1. Equation (3. 39) is written for all y points along an x axis, and the values of $C_{i,j,k+1}$ are determined by a simultaneous solution of the series of equations.

Stability analyses by Douglas [1961] and Richtmyer [1959] show that the above equations are stable for any value of r. This has led many people desirous of using numerical solutions to concentrate on implicit solutions, so as to escape the limitations of explicit solutions. Smith [1965] states that any use of a value of r greater than unity is an inaccurate approximation of $\frac{\partial c}{\partial t}$. A value of r greater than unity can easily result in instabilities at the extreme ends of the concentration distribution. These instabilities are especially noticable during the early stages of the computational process, i.e., for small values of t. Shamir and Harleman [1967] suggest the use of small values of Δt initially and then progressively larger values of Δt as t becomes larger. Much of the computational experience reported in the literature demonstrates that the solutions using implicit procedures are not unconditionally stable and that smaller values of r should be used so that $\frac{\partial c}{\partial t}$ can be more accurately approximated. In view of the time consuming process needed to solve Equations (3.38) and (3.39), values of r in the range of unity negate the advantages of using implicit methods.

Stone and Brian [1963] presented an additional problem which occurs when using either explicit or implicit numerical procedures for convective dispersion problems. Numerical models capable of handling both diffusion and convection remain stable whenever the convection becomes zero. Stone and Brian demonstrated that whenever the diffusion became zero and convection remained, oscillations occurred and a "pseudo" diffusion is present, thus, presenting the problem of induced numerical dispersion. To overcome this problem, they suggest the application of weighting coefficients to an implicit approximation. Regrettably, the weighting factors do not eliminate the oscillations; they only reduce their magnitude.

Errors within the computations are to be expected whenever Δx, Δy and Δt are finite values. The attitude of the user to finite difference techniques should be that of (1) avoiding approximations which are grossly inaccurate or which produce oscillation and (2) utilizing techniques which allow for an estimation of the magnitude of the errors. An example of the latter is the estimation of the true solution by consecutive solutions using successively smaller values of Δx, Δy and Δt. If a solution is found and noted at a particular y and t and is plotted against the step size Δx, Δy or Δt on an arithmetic graph, and if the step size for consecutive solutions is successively reduced and computations made for the solution at the same x, y and t, then the values of the solutions should converge to the value of the true solution. By the above procedure, the knowledge of the existence of errors is of beneficial use. Such analyses, however, do not reduce the errors and require much computational effort. Finite difference procedures as error free as possible are to be sought.

3-4d Characteristic Solution. Garder, Peaceman and Pozzi [1964], while studying convective dispersion in porous media for problems of the petroleum industry, developed a new and unique method to solve the convective dispersion equation. For the dispersion equation with two dimensional convection they made use of the hyperbolic nature of the first order differentials to develop equations for characteristic lines. In the process of developing the characteristic equations, the convective terms are separated from the diffusion terms. Thus, for their problem a series of three equations is formed, one equation expressing diffusion and two equations expressing convection for each of the two directions. To solve the system of equations they used two grid networks, one to approximate the convection and the other to solve the diffusion equation. Garder, et al concluded that the method was accurate and that the solution agreed with their experimental data.

Using the two dimensional convective diffusion equation of this study, the following analysis is made to separate a characteristic from

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = E_X\frac{\partial^2 C}{\partial x^2} + E_Y\frac{\partial^2 C}{\partial y^2} \qquad (3.3)$$

Consider a value F such that

$$F = E_x\frac{\partial^2 C}{\partial x^2} + E_Y\frac{\partial^2 C}{\partial y^2} \qquad (3.40)$$

then Equation (3. 3) becomes

$$u\frac{\partial C}{\partial X} + \frac{\partial C}{\partial t} - F = 0 \qquad (3.41)$$

By the chain rule dC may be expanded such that

$$dC = \left(\frac{\partial C}{\partial X}\right)dx + \left(\frac{\partial C}{\partial t}\right)dt \qquad (3.42)$$

Thus, $\frac{\partial c}{\partial t}$ may be expressed by Equation (3.41) as

$$\frac{\partial c}{\partial t} = \left(dc - \frac{\partial c}{\partial x}dx\right)/dt \tag{3.43}$$

Substituting Equation (3.43) into Equation (3.41) yields

$$u\frac{\partial c}{\partial x}dt + dc - \frac{\partial c}{\partial x}dx - Fdt = 0 \tag{3.44}$$

which can be rearranged into

$$\frac{\partial c}{\partial x}(u\,dt - dx) + dc - Fdt = 0 \tag{3.45}$$

From the above relationship, a line in x-t space may be selected such that

$$u\,dt - dx = 0 \tag{3.46}$$

or

$$\frac{dx}{dt} = u \tag{3.47}$$

Substituting the selection, Equation (3.46), into Equation (3.45) yields

$$dc - Fdt = 0 \tag{3.48}$$

or

$$\frac{\partial c}{\partial t} = E_x\frac{\partial^2 c}{\partial x^2} + E_y\frac{\partial^2 c}{\partial y^2} \tag{3.49}$$

Thus, it is demonstrated that the convective diffusion phenomenon described by Equation (3.3) can be described by Equations (3.47) and (3.49).

The method of characteristics allows the two dimensional diffusion equation

$$\frac{\partial c}{\partial t} = E_x \frac{\partial^2 c}{\partial x^2} + E_y \frac{\partial^2 c}{\partial y^2} \qquad (3.49)$$

to be integrated along the characteristic line

$$\frac{dx}{dt} = u \qquad (3.47)$$

The integration of the diffusion equation along a characteristic line can be handled by a variety of techniques. As previously mentioned, Garder, et al [1964] used two grid systems, one a moving system to approximate convection, and the other, a stationary system to solve the diffusion equation. The two grid systems are necessary to solve their problem because unsteady velocities are included, and concentrations are convected differenct distances when unsteady flows occur. Several approximations had to be used for proper interpretation of convection and to make the necessary transpositions between grid systems. Garder, et al found that these approximations did not affect their results and that their model was accurate over a large range of values.

As the velocities used in this study are uniform, steady and unidirectional, only one grid network would be necessary if the proper conditions could be met. The use of only one grid network would eliminate the use of the approximations used by Garder, et al To use only one grid, it is necessary that concentration values be moved by convection from one grid point to the exact location of another grid point. The concentration at each lateral point, y, is displaced a distance

$$dx = u(y)\,dt \tag{3.50}$$

where u(y) is the velocity in the x direction for the lateral position y. The distance dx must be equal to the grid increment Δx or to some multiple of Δx. Often, a velocity distribution must be contrived or adjusted to meet the criterion. The changes are minor if proper attention is given to the initial construction of the computational grid. This criterion enables the characteristic solution to be used in a more exact manner.

The procedure for the solution of the diffusion equation can be applied either before or after the solution of convection. Either the explicit procedure or the implicit procedure may be used. Stability and convergence criteria remain identical to those of the explicit or implicit solution of the two dimensional diffusion equation. It should be noted that if the explicit procedure is used, there is no limitation upon Δx by Equation (3.32) as the convection term has been eliminated by the method of characteristics. Thus, for using the explicit method in a solution by characteristics the only limiting criterion is

$$\Delta t < \frac{\overline{\Delta x}^2 \cdot \overline{\Delta y}^2}{2(E_x \overline{\Delta y}^2 + E_y \overline{\Delta x}^2)} \tag{3.33}$$

The bothersome limitation on Δx has been eliminated, and a more reasonably spaced computational grid may be constructed.

At this time, the similarity should be noted between the approximate numerical model of Fischer [1966] and the solution along characteristic lines. Both procedures may be interpreted physically as allowing for diffusion and then for a displacement proportional to the local velocity.

To gain computational experience, the explicit, implicit, and characteristic solutions were programmed for the digital computer. The development of these models is presented in the following chapter.

Chapter 4

DEVELOPMENT OF THE COMPUTATIONAL ALGORITHMS

4-1 Lateral Boundary Conditions

Most two dimensional convective dispersion problems are bounded in the transverse direction. When lateral boundaries exist, no transport can occur across the boundary, and thus, at each of the transverse boundaries

$$\frac{\partial c}{\partial y} = 0 \qquad (4.1)$$

The requirement imposed by Equation (4. 1) can be interpreted numerically by either an expansion by Taylor's series or an image concept.

An evaluation by Taylor's series of points adjacent to the boundary enables a point on the boundary, j=b, to be described by two points adjacent to the boundary, j=b±1 and b±2, in the following manner

$$3C_{i,b,k+1} = 4C_{i,b\pm1,k+1} - C_{i,b\pm2} - 2\Delta y\left(\frac{\partial c}{\partial y}\right)_{i,b,k+1} + O(\overline{\Delta y}^3) \qquad (4.2)$$

where $\left(\frac{\partial c}{\partial y}\right)_{i,b,k+1}$ is the gradient at the boundary and $O(\overline{\Delta y}^3)$ is the magnitude of the error. Thus, for $\frac{\partial c}{\partial y} = 0$ at j=b, a simple relationship exists. In an explicit algorithm, the Taylor's series interpretation is applied by evaluating C_{k+1} at all interior points. The values of the interior points adjacent to the lateral boundary are used to compute the value of C_{k+1} at the lateral boundary. This scheme was tried in both explicit and implicit models and was found to yield results not as accurate as the following method.

Equation (4.1) is often physically interpreted as an image condition or as a reflection condition. Although the image condition is sometimes considered a mathematical artifact, its proper usage can produce accurate results. The image concept may be used by placing a boundary midway between two points, so that one point is within the grid's interior at $\Delta y/2$ and the other point, the image point, is outside of the boundary at $\Delta y/2$. If the two points are equivalent in value, diffusion cannot occur between the two points, and

$$C_{i,b,k+1} = C_{i,b\pm1,k+1} \tag{4.3}$$

where j=b refers to the exterior point and j=b±1 refers to the interior point. This concept is applied by computing the values of C for all interior points, and then setting the exterior points to be equal in magnitude to their adjacent interior points. This image concept was tried in both explicit and implicit models and found to be more accurate and more stable than the Taylor series approximation. In addition, the image concept was computationally simple to apply.

4-2 Longitudinal Boundary Conditions

The longitudinal boundaries present a problem for numerical interpretation. For the solution of a general problem where longitudinal boundaries have no effects upon diffusion, the longitudinal boundaries are assumed to be at an infinite distance from the source. To solve a numerical problem a finite distance for the position of the boundaries must be assumed such that a semi-infinite condition exists where no reflective effects are produced by either boundary. The most desirable way to model semi-infinite boundaries is to construct a grid system large enough in longitudinal extent so that no diffusive effects ever reach the edge of the grid system. Unfortunately, this approach requires tremendous amounts of computer storage which is often unavailable. Thus, it becomes necessary to develop an artificial boundary such that diffusive effects will be accurately transmitted through the boundary.

The artificial boundary is constructed by estimating the concentration value for the points at each longitudinal edge of the grid system. If the value of the concentration at the point is assumed to be zero, an artificial sink is created at the boundary, thus causing the slope of the gradient to be artificially steeper as it approaches the boundary. Consequently, it is necessary to preserve the proper gradient at the longitudinal edges of the grid system. The most elementary manner of creating the proper boundary condition is to let the slope between the last two increments remain constant, i. e.,

$$\left(\frac{\partial c}{\partial x}\right)_{b,j,k+1} = \left(\frac{\partial c}{\partial x}\right)_{b+1,j,k+1} \qquad (4.4)$$

Figure (4. 1) illustrates this condition. By this analysis

$$C_{1,j,k+1} = 2C_{2,j,k+1} - C_{3,j\,k+1} \qquad (4.5)$$

The above formulation was tested in an explicit model by processing a contrived problem on an extra long longitudinal grid so that no diffusive effects reached the boundary. Then, the problem was processed again with a new boundary established well within the range of diffusive effects. The values of the concentrations were significantly different from the original processing. The concentration values for points near the boundary had the maximum error, and the points near the maximum concentration had the least error. The only agreement between the values of the two processings was the consistency to produce accuracy in the first significant figure.

The discrepancy between the values of the two processings is due to the variability in the slope of the concentration gradient. For pure diffusive effects the distribution resembles a normal distribution where the slope is constantly changing. To approximate the concentration value at the boundary, several schemes involving difference tables were tried. The most successful approximation was obtained by a form of a difference table which utilizes the concentration values of four points adjacent to the boundary to approximate the concentration at the boundary. Figure (4. 2) illustrates these points and their associated concentrations.

Finite difference tables are constructed from a list of independent variables, denoted under position column in Table (4. 1), and dependent

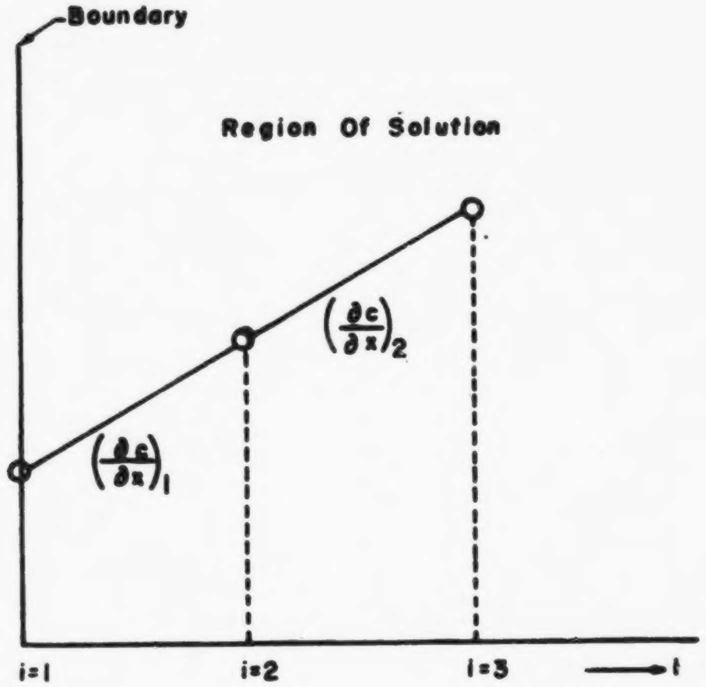
Boundary
Region Of Solution
$\left(\frac{\partial c}{\partial x}\right)_1$
$\left(\frac{\partial c}{\partial x}\right)_2$
i=1
i=2
i=3
i

FIGURE 4-1 SIMPLE TRANSMISSION BOUNDARY CONDITION

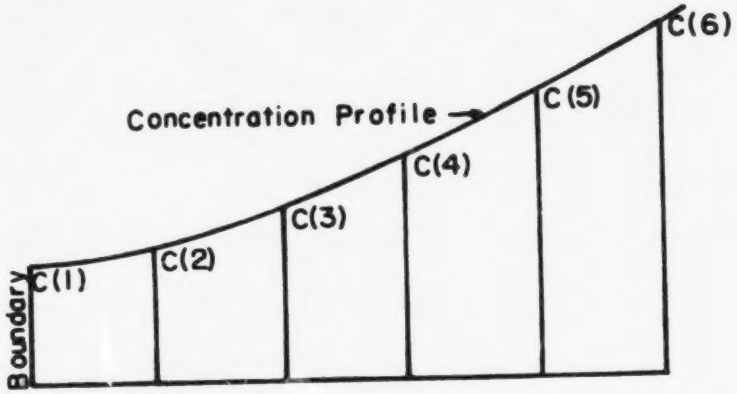

FIGURE 4-2 TYPICAL CONCENTRATION PROFILE NEAR LONGITUDINAL BOUNDARY

Values Known to Exist

Values to be Approximated

Position	Concentration		
X=1	C(1)	$DC_0=?$	$\Delta C_0=?$
X=2	C(2)	$DC_1=\frac{C(3)}{C(2)}$	
X=3	C(3)	$DC_2=\frac{C(4)}{C(3)}$	$\Delta C_1=DC_2-DC_1$
X=4	C(4)	$DC_3=\frac{C(5)}{C(4)}$	$\Delta C_2=DC_3-DC_2$
X=5	C(5)		

Summary of Steps Necessary to Approximate C(1)

1. $\Delta C_0 = \Delta DC_2 - \Delta DC_1$
2. $DC_0 = DC_1 + |\Delta C_0|$
3. $C(1) = C(2)/DC_0$

TABLE 4-1 DIFFERENCE TABLE FORM USED TO APPROXIMATE CONCENTRATION AT BOUNDARY

variables, denoted under concentration column in Table (4. 1). Finite difference tables are used for interpolation, extrapolation and error analysis by establishing the relationship, if any, of the dependent variable to the independent variable. Finite difference tables establish relationships by using a series of successive subtractions. Along the rising section of the concentration profile such as that illustrated in Figure (4. 2), there is a percentage decrease of concentration as determined by the values DC,the third column of Table (4. 1). The percent decrease, DC, progressively decreases in value and is determined by the values ΔC. The values of ΔC are then used to establish the relationship between C(2) and C(1) by a series of steps illustrated in Table (4. 1). It should be noted and emphasized that there is no theoretical basis for this approximation. The approximation was tested in the same manner as the previous approximation, and it was found that the approximation was consistently accurate to three or more significant figures.

4-3 Initial Conditions

For the initial conditions of the moving fluid medium, a situation typical of problems of Taylor [1954] and Fischer [1966a] was selected. Thus, the concentration is zero at t=0 throughout the grid system except at the point of injection of the conservative tracer material. At the point of injection, the concentration applied is unity. By using a value of unity the concentrations at grid points are expressed in the percentages of the initial concentration. Additionally, the sum of the concentration distribution is unity.

The works of Taylor and Fischer were concerned with the dispersion of dye from an instantaneous slug injection of material uniformly mixed over a cross sectional area. This, in effect, is injection along the surface of a plane. Admittedly, most injections into moving fluids are neither instantaneous nor completely mixed over a plane but are continuous for a finite period of time and are injected either as a point source or along a line source. Nevertheless, the solution of this problem is a good reference for actual conditions, and it allows the accuracy of the method to be checked by the works of others. After this fundamental formulation is adequately solved, other types of injection sequences can be tried by future workers.

4-4 Algorithms

4-4a Explicit Model. The explicit model is based upon a forward finite difference interpretation of the two dimensional convective diffusion equation by using the explicit operator, Equation (3. 27). The molecule for the explicit operator is given in Figure (3. 2), and the entire computer program of the explicit method is presented in Appendix A.

After the input data is processed and internal program functions are zeroed, a check is made of stability requirements for the increment sizes. If a velocity exists, ΔX is checked for stability by Equation (3. 32). If no velocity is present, no bound exists upon the grid limitation. When the step size ΔX does not meet the requirements, the step size is changed to meet the requirement of Equation (3. 32). After stability conditions have been met for ΔX, the size of Δt is checked by Equation (3. 33). If the stability condition is not met, a new value of Δt is calculated by Equation (3. 33). The checking and changing of ΔX and Δt insures that the computations will meet stability conditions at all times.

When stability has been assured, the concentration values for all internal grid points are computed using the explicit operator, Equation (3. 27). Using the values of concentration for the internal grid points, the boundary conditions are satisfied by the previously described procedures. That is, the lateral boundaries are satisfied by the image condition, Equation (4. 3), and the longitudinal boundaries are satisfied by the approximation procedure of Table (4. 1). After all concentration values have been computed for all points in the grid system, the dispersive parameters are computed along each streamtube equivalent, y. A discussion of the dispersive parameters follows in a later section. After all computations have been performed for concentrations and dispersive parameters, the process proceeds to the next time increment. Interpretive results of the explicit model are provided in the next chapter.

4-4b Implicit Model. The implicit model is based upon the Crank-Nicolson finite difference interpretation of the two dimensional convective diffusion equation. The molecule for the implicit operator is given in Figure (3. 3), and the entire computer program is presented in Appendix B. The basic framework of the implicit model is similar to that of the explicit model with the exception of stability conditions, computation of concentrations and boundary approximations.

As the implicit model is unconditionally stable by theoretical analysis, there is no need for stability checks upon Δx and Δt. The suggestion of Smith [1965] should again be noted, i. e., $r = \Delta t/\Delta x^2$ should not be larger than unity or inaccurate approximations of $\partial c/\partial t$ will occur. While debugging the computer program of the implicit model, it was found that the best results using the implicit model occurred when the value of r was less than one-half.

To compute the values of the concentrations, the procedure outlined by Douglas [1961] was used. The procedure is the consecutive solution, first, of Equation (3. 38) and, second, of Equation (3. 39). The solution of Equation (3. 38) involves an approximation of the concentration values at time $t+\Delta t$ by using the Crank-Nicolson approximations for the derivatives in the x direction only. Within the computer program, these values are labeled CX. As the expression of the values of CX contains three unknowns, the simultaneous expression of the equations along a streamtube, y, produces a tridiagonal matrix. This matrix is easily solved simultaneously by Gaussian elimination, Fox [1965], for all CX terms. These values of CX are then used in the solution of Equation (3. 39). Equation (3. 39) includes the Crank-Nicolson approximation of the derivatives in the y direction. The unknown values at time are labeled CY within the computer program. Again, the formulation of the equations along a line of constant x, normal to y, produces a tridiagonal matrix which is solved simultaneously by Gaussian elimination.

Computational experience shows the interpretation of longitudinal boundary conditions to be extremely important for the implicit model. The matrix techniques of the implicit model make it necessary to include the equations for the longitudinal ends within the initial matrix formulation. The simple expression for the continuation of the slope, Equation (4. 5), was used initially. Its usage provided excellent results whenever plug flow conditions were being tested in the model. But whenever shear flow conditions were tested, severe oscillations developed at each longitudinal end and soon destroyed the concentration distributions. The oscillations are reduced in magnitude, but not eliminated, by using the approximation of Equation (4. 5) in the matrix formulation, and then recomputing the end point concentrations by the procedure of Table (4. 1). Several other approximations were tried, including a Taylor series expansion and a continuation of the second partial derivative of C, but they proved to be little better than the usage of Equation (4. 5).

4-4c Characteristic Model. The characteristic model is based upon the separation of the two dimensional convective dispersion equation into an equation for diffusion and an equation for convection. The development of the two equations is described in Chapter 3, and the equations to be utilized in the model are Equations (3. 48) and (3. 50). The solution of the two equations is obtained by integrating the diffusion equation, either implicitly or explicitly, along the characteristic line which represents the convection. The selection and development of a method to perform this integration is presented in this section. The complete form of the computer program is presented in Appendix C. As the basic framework of the program is the same as that of the explicit and implicit models, only the calculation of concentration values using the method of characteristics will be discussed here.

Although the integration of the diffusion equation along a characteristic line implies a one step procedure, the process can be handled by the two step procedure of solving first one equation and then the other equation. Procedures with each equation being solved first were programmed. For plug flow conditions, no differences in the results were found. For shear flow conditions, however, the solutions converged one step sooner when the convection equation was solved first. Thus, the procedure selected was to solve the convection equation, Equation (3. 51), for every y position at time t, and then to solve the diffusion equation, Equation (3. 50), for concentration values at time $t+\Delta t$.

The solution of the convection equation is handicapped in that the displacement distance, $\Delta x_d = u(y) \cdot \Delta t$, may not always be equal to the step increment, ΔX. Thus, a certain amount of manipulation is necessary. Garder, et. al. [1964] let the displacement distances, ΔX_d remain between grid points and, then, used a summation and interpolation analysis to find the values of concentration at the grid points. In as much as velocity determinations are seldom exact but are averaged values even for point measurements, the velocity distributions can be manipulated so that the displacement distances, ΔX_d , are equal to the grid increment,

Δx, or some multiple of the grid increment. To achieve this condition, it is necessary to contrive a common multiple for the velocity distribution. The applicability of this concept will be illustrated in example problems in the following chapter.

Concentrations along a constant lateral distance, y, are characterized by a velocity, u(y). Each concentration is displaced longitudinally a distance $u(y) \cdot \Delta t$ for each time step. The calculation of the displacement increment is included in the computer program as IDC(y). As concentration values are convected in the direction of the velocity, some are convected beyond the downstream longitudinal boundary and are neglected in subsequent calculations. However, for each point convected off of the grid a void is created at the opposite end. This void can only be filled by the extrapolation of existing values. The concept illustrated in Table (4. 1) is used to fill the void by modifying the procedure so that the values are extrapolated to more than one point whenever necessary. The extrapolated values being in a direction opposite to that of the flow are low and their effects minimal. Their effects can be further decreased by increasing the extent of the grid system.

As shown in the next chapter, the explicit method is accurate whenever convection is not included in the diffusion computations. Also, the explicit method is simpler to apply than the implicit method. Therefore, the explicit method was selected to solve the diffusion equation, Equation (3. 50), and Figure (3. 1) is again applicable to the procedure followed.

Using the explicit method to solve the two dimensional diffusion equation establishes the existence of the same stability criteria as exist for all explicit methods. The primary advantage of the characteristic concept is the elimination of the velocity term from diffusion computations. This eliminates the restraint on the grid increment ΔX. Therefore, the only stability criterion applicable is that on the time step Δt, Equation (3. 33).

The computer program includes a routine to set the size of consistent with making $u(y) \cdot \Delta t$ equal to ΔX. If Δt cannot be made consistent between the above condition and Equation (3. 33), then ΔX is changed such that these conditions will be met if possible. As the routine will try to set Δt as large as possible consistent with stability, a value S was included within the program so that a value of Δt will be set at stability divided by S. This allows for interpretations of the convergence of the explicit method. These interpretations are illustrated in the following chapter.

4-5 Dispersive Parameters

The coefficient of diffusion was first related to the variance of the concentration distribution by Einstein [1905] and is determined by

$$D = \frac{1}{2} \frac{d\sigma_s^2}{dt} \qquad (4.4)$$

where σ_s^2 is the variance of the spatial distribution in the s direction, t is the time, and D is the coefficient of diffusion. By this definition, the diffusion coefficient may be determined from the variances of two spatial distributions, σ_s, in the s direction, one at time t_1 and the other at time

t_2. That is, the diffusion coefficient can be determined from

$$D = \frac{1}{2} \frac{\sigma_{s_2}^2 - \sigma_{s_1}^2}{t_2 - t_1} \qquad (4.5)$$

This same relationship is used to determine the dispersion coefficient whenever dispersive effects exist with diffusion. Equation (4. 5) is impractical to use on measured experimental data because of the difficulty in acquiring accurate spatial concentration distributions for any given time.

Fischer [1966b] showed that a dispersion coefficient can be determined from the temporal variance of a dispersive plume measured at two given points over a varying time period. The mean convective velocity and the time of passage of the centroid of the distribution for each station are needed to use in

$$E_T = \frac{1}{2} \bar{u}^2 \frac{\sigma_{t_2}^2 - \sigma_{t_1}^2}{\bar{t}_2 - \bar{t}_1} \qquad (4.6)$$

where E_T is the dispersion coefficient, $\bar{u}$ is the mean velocity, σ_t^2 is the variance of the temporal distribution, $\bar{t}$ is the time at the passage of the centroid, and the subscripts 1 and 2 refer to the two measuring stations.

For the purposes of this study, the coefficient determined by Equation (4. 5) is used because the spatial concentration distributions are readily available at each time step. For each time step within the computer program, the position of the centroid, the variance and the standard deviation are calculated from the concentration distributions. The value of the variance from the preceding time step is stored so that the dispersion coefficient can be computed at each time increment.

In addition, other statistical parameters are calculated and printed to make interpretations about changes of the distribution curves between time steps. As analytical solutions of the diffusion equation, Equations (3. 6) and (3. 8) resemble the normal or Gaussian probability distribution, the statistical parameters of variance, skewness and peakedness and their relationship to the normal distribution can be used to describe changes occuring within the distribution. The skewness and the peakedness are evaluated by computing the third and fourth moments about the centroid. For a normal distribution, the skewness is zero and the peakedness is three. Parratt [1961] defined a precision index, P. I., which is a combination of skewness and peakedness and weights their relative deviation from the normal distribution by

$$\text{P.I.} = 3(\text{skewness})^2 - 2\ \text{Peakedness} + 6.$$

P. I. is zero for a normal distribution, positive for a skewed distribution and negative for an extremely peaked distribution. The parameters of skewness, peakedness and precision index can be used to make only the most general of inferences about the changes of the shape of the concentration distribution with time.

No interpretations were made of the data produced by the above statistical parameters. As will be shown in the next chapter, different numerical techniques produce different results and the initial steps are seldom accurate. Thus, if the dispersion coefficients are questionable, then interpretations of concentration distributions would be meaningless. It is helpful, however, to have the statistical parameters in the program, as they can define the changes within the concentration distributions with succeeding time steps.

The decrease of the maximum concentration with time is a parameter which is important in pollution studies. This should be easily defined by determining the highest concentration from the concentration distribution. But if the mode of the distribution does not fall exactly upon a grid point, the highest concentration value is in error as a peak concentration value. Whenever the peak value is between two grid points, a computational routine is available within the program to estimate the peak value by Lagranian interpolation, Kunz [1957], using a third order curve through four points, two points on each side of the peak. The accuracy of this estimating procedure is unknown, and thus, this approximation should only be used for estimates.

Chapter 5

COMPARISON OF COMPUTATIONAL ALGORITHMS

5-1 Plug Flow Test Problem

The plug flow problem as formulated above is an excellent problem to test the models. While the models are constructed to handle two dimensional diffusion and unidirectional convection, the plug flow problem consists of diffusion and convection for the x direction only. As there is no velocity variation over a cross section, convective dispersion cannot occur. Also, if the tracer material is applied uniformly over the cross section as a plane source, no lateral gradient of concentration exists, and no net transport in the lateral, y, direction can occur. The solution to the plug flow problem as formulated is

$$\frac{C}{C_o} = \frac{1}{\sqrt{4\pi E_x t}} \exp\left[-(x-\bar{u}t)^2/4E_x t\right] \qquad (3.8)$$

The concentration profiles of the plug flow problem as computed by the models can be checked against the concentration distributions of Equation (3.8). As convective dispersion does not exist and only longitudinal diffusion does exist, then any dispersion coefficient calculated from the plug flow concentration distributions produced by the models should be the same as the diffusion coefficient used in the computations. These checks on the concentration distribution and the diffusion coefficient provide an excellent evaluation of the models.

For the test problem, values for each variable were selected which would be typical of the order of magnitude of the variable in naturally occurring problems. A coefficient of longitudinal turbulent diffusion was chosen as 0.0025 square feet per second; this value was also used as a lateral coefficient. A velocity of 0.05 feet per second was selected as being typical of a slowly moving fluid. The data are applied to steady, uniform flow in a long, straight channel with no secondary flows.

The explicit model, being the first model developed, was thoroughly tested on the plug flow problem. For the test data, the limitations on the step sizes of Δx and Δt were set by the computer program to be $\Delta x = 0.09$ feet and $\Delta t = 0.8$ seconds. These are the maximum values which will meet the stability requirements of Equations (3.32) and (3.33).

The explicit model was tested on two different types of coordinate systems, one a stationary system and the other a moving system. For the stationary system a distance from the source is assigned to each point, and these distances never change. For the moving coordinate system a value of distance from the centroid of the concentration distribution is assigned to each grid point. The distance from the centroid never changes, but distance from the point of injection changes for each time step. The moving coordinate system is described by ξ where

$$\xi = x - ut \qquad (5.1)$$

and x is the original distance from the point of injection, u is the steady, uniform velocity, and t is the time since injection. For an accurate method, no differences should be detected between values obtained from each coordinate system.

Several differences are noted between the results of solutions using the two coordinate systems in the explicit model. The results from the stationary coordinate system show skewness developing at the first step and a lower value for the standard deviation being computed. Figures (5. 1) and (5. 2) show the difference in the distributions for times equal to 10. 4 seconds and 100 seconds. A probability scale is used to plot the data since the concentration distirubtions resemble normal distributions. As the results of the moving coordinate system plot as a straight line, the concentration distribution for the moving coordinate system is normally distributed.

For the moving coordinate system the calculated dispersion coefficient, based on the values of the standard deviation, is 0. 0025 square feet per second. Thus, the same value was calculated as was used for the calculations, and the explicit procedure is accurate when no convection terms are included within the computations. For the stationary coordinate system, the dispersion coefficient was computed to be 0. 0015 square feet per second when $\Delta x = 0.09$ feet and $\Delta t = 0.80$ seconds. The dispersion coefficient has an error of 40%. To investigate the nature of the error, the time step Δt was halved for each succeeding time the data was processed.

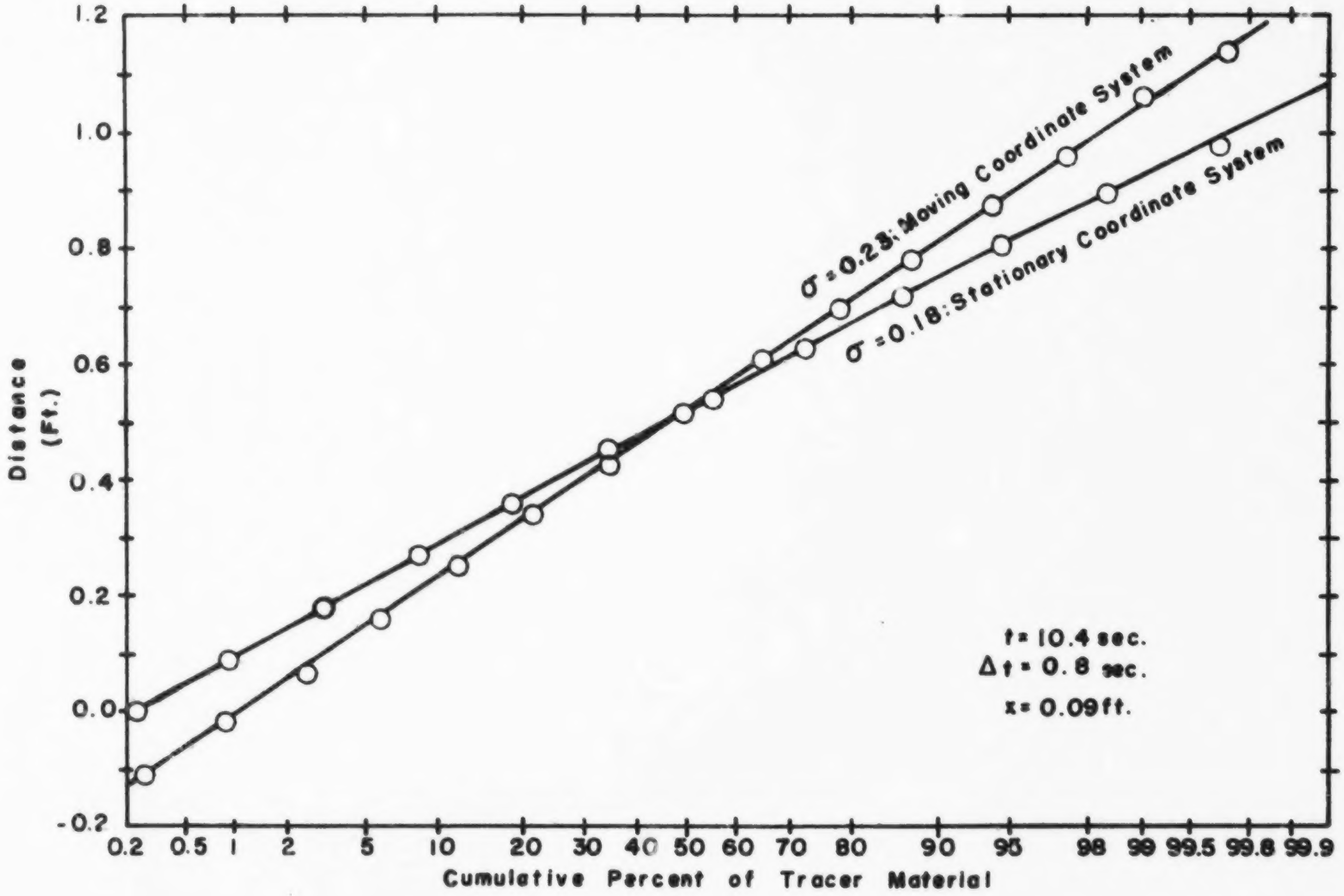

FIGURE 5-1 COMPARISON OF COORDINATE SYSTEMS FOR EXPLICIT METHOD AT TIME = 10.4 sec.

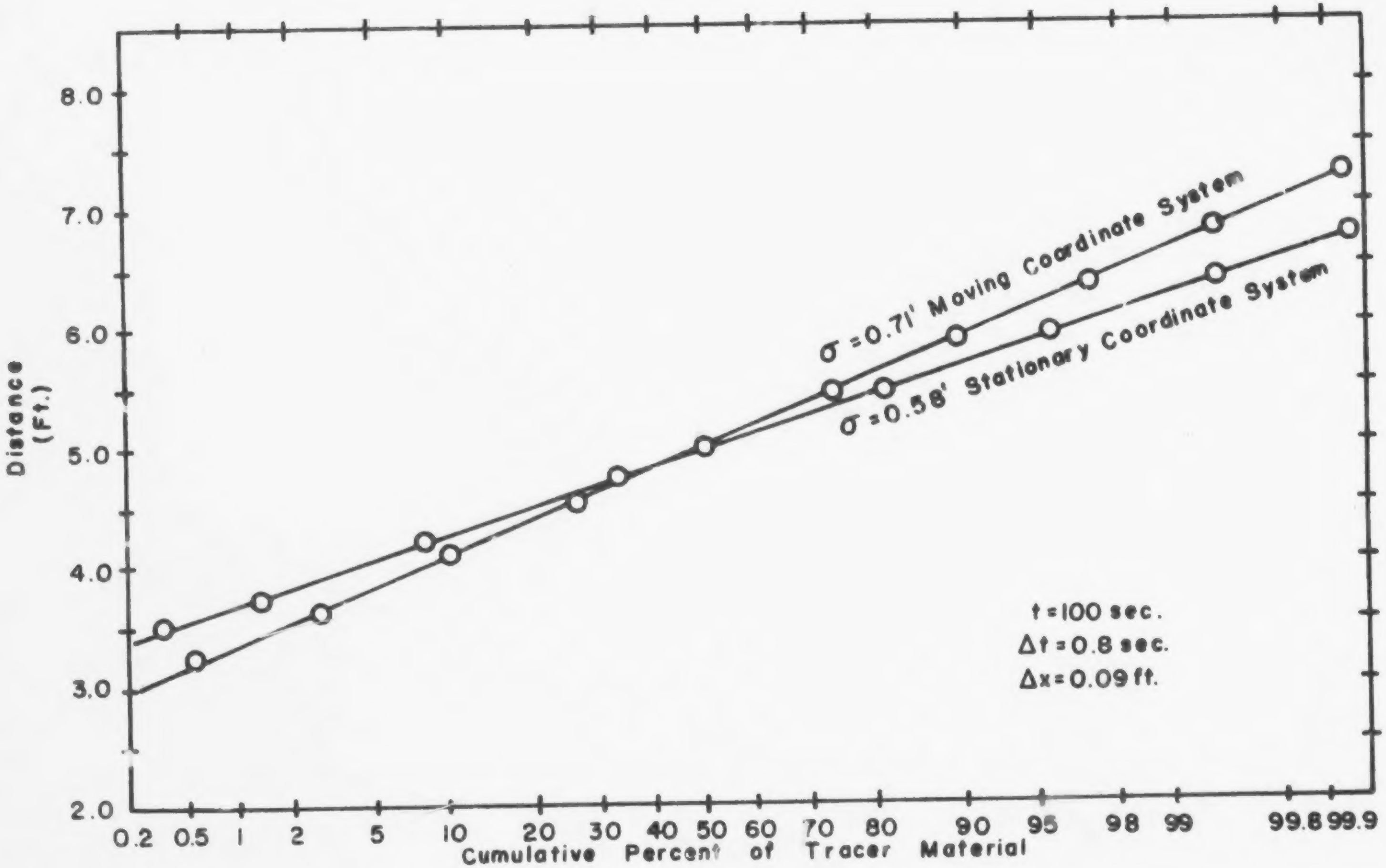

FIGURE 5-2 COMPARISON OF COORDINATE SYSTEMS FOR EXPLICIT METHODS AT TIME = 100sec.

As the calculated dispersion coefficient is constant for a given set of increment sizes under plug flow conditions, no graphical analyses of the dispersion coefficient were performed as only straight horizontal lines would result. Instead, graphical analyses were performed on the standard deviation. The significance of the standard deviation is twofold. First, it is the primary value used to compute the diffusion coefficient. Second, it describes the movement of a point on the concentration distribution; a point that represents the spread of 68.3% of the diffusing material. Substituting the value of σ for $x-\bar{u}t$ in the exponent of Equation (3.8) and relating the value of σ to t, the value of t is proportional to σ^2, or stated differently, the value of σ is proportional to $t^{1/2}$. For a graph on paper with logarithmic scales with σ as abscissa and t as ordinate, the relationship should plot as a straight line with a slope of one half. Figure (5.3) illustrates the accuracy of the above analysis, as all lines have a slope of one half.

Figure (5.3) contains the graphs of σ versus t for three solutions by the explicit model with different values of Δt. The interesting part of Figure (5.3) is the parallelism of the three lines. Thus, the values of the standard deviation do not vary in a manner that would eventually lead to the correct solution, and the standard deviations remain incorrect by constant values of log σ. If the values of the dispersion coefficient produced by the three increments are plotted arithmetically against the time step, Figure (5.4), insight to the variability of the error in the dispersion coefficient is gained. No finite value of Δt will reproduce an

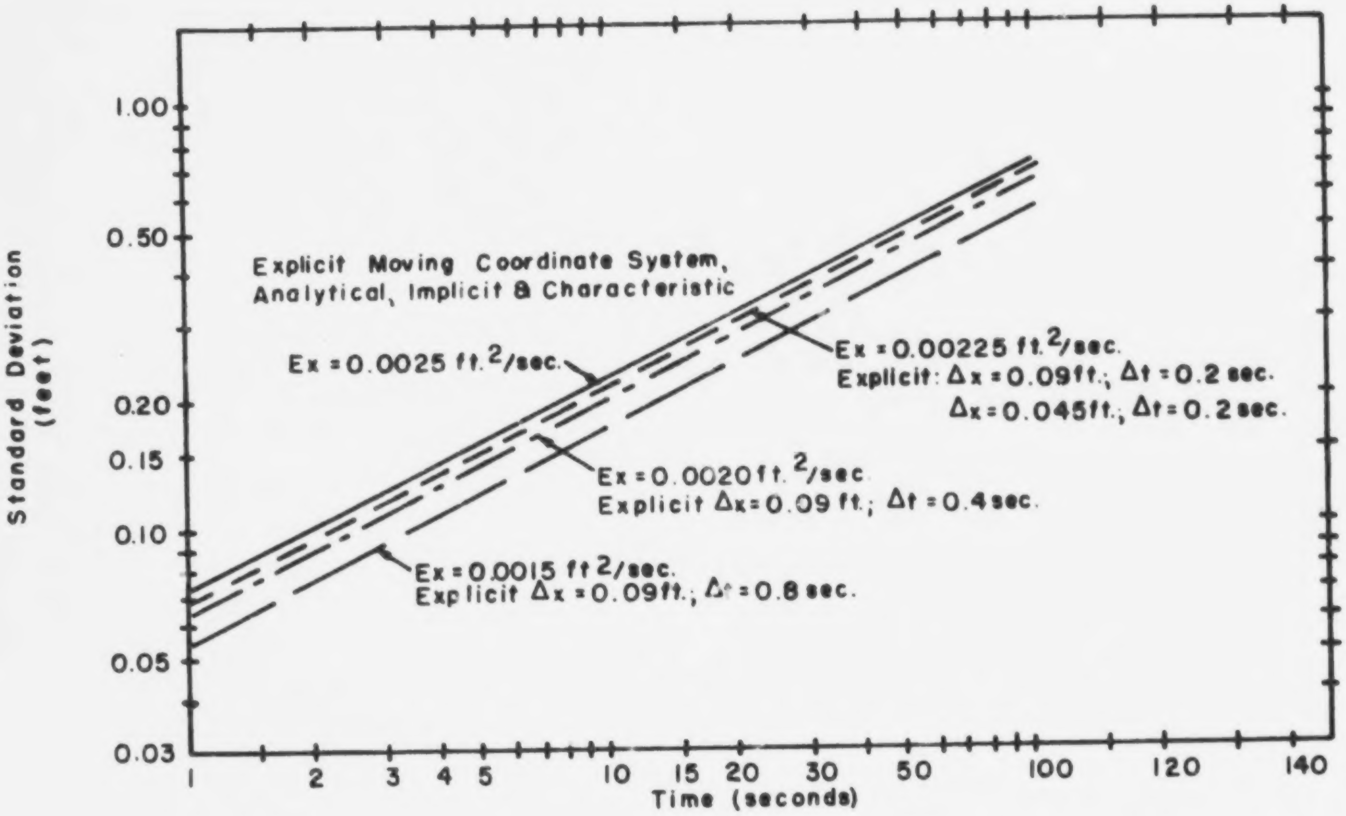

FIGURE 5-3 STANDARD DEVIATION VERSUS TIME FOR PLUG FLOW PROBLEM

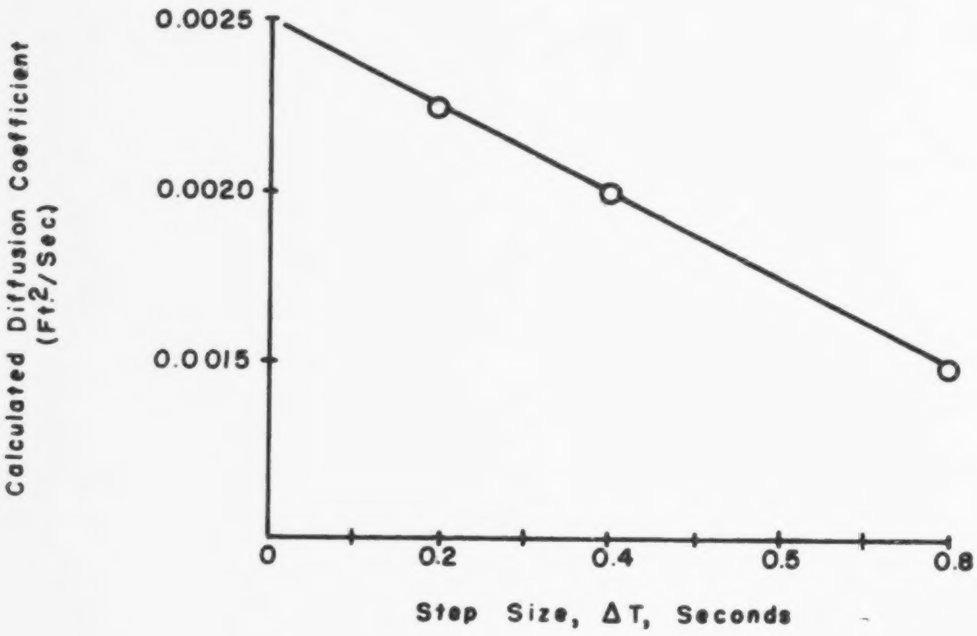

FIGURE 5 - 4 CALCULATED DISPERSION COEFFICIENTS VERSUS TIME INCREMENT SIZE FOR PLUG FLOW

exact value of the dispersion coefficient, and only an impractically small value of Δt will yield a value less than 5% in error. Note that this condition exists for only the stationary coordinate system when the convection term is included within the model.

The decrease in maximum concentrations for the explicit models with the stationary coordinate system is presented in Figure (5. 5) along with the results of the analytical solution and the moving coordinate system which are the same. The value of C_{max}/C_o is the initial concentration, has a slope of minus one half when plotted against t on a graph with logarithmic scales. For pure diffusion, this can be shown to be true from an analysis of Equation (3. 8). Figure (5. 5) again shows straight lines produced by each of the three step sizes with the variations between the parallel lines again being constant. The constant difference in lines can be attributed to the effects of the standard deviation. When the standard deviation of the concentration distribution is lower, the peak value of the concentration must be greater.

The existence of the errors in the explicit method recalls the discussion by Stone and Brian [1961] which was presented in the discussion of the implicit method in Chapter 3. As noted there, induced numerical dispersion or "pseudo" dispersion can become a major problem whenever convection and diffusion are combined in a finite difference model. Apparently, this is the source of the error within the explicit model when using the stationary grid system.

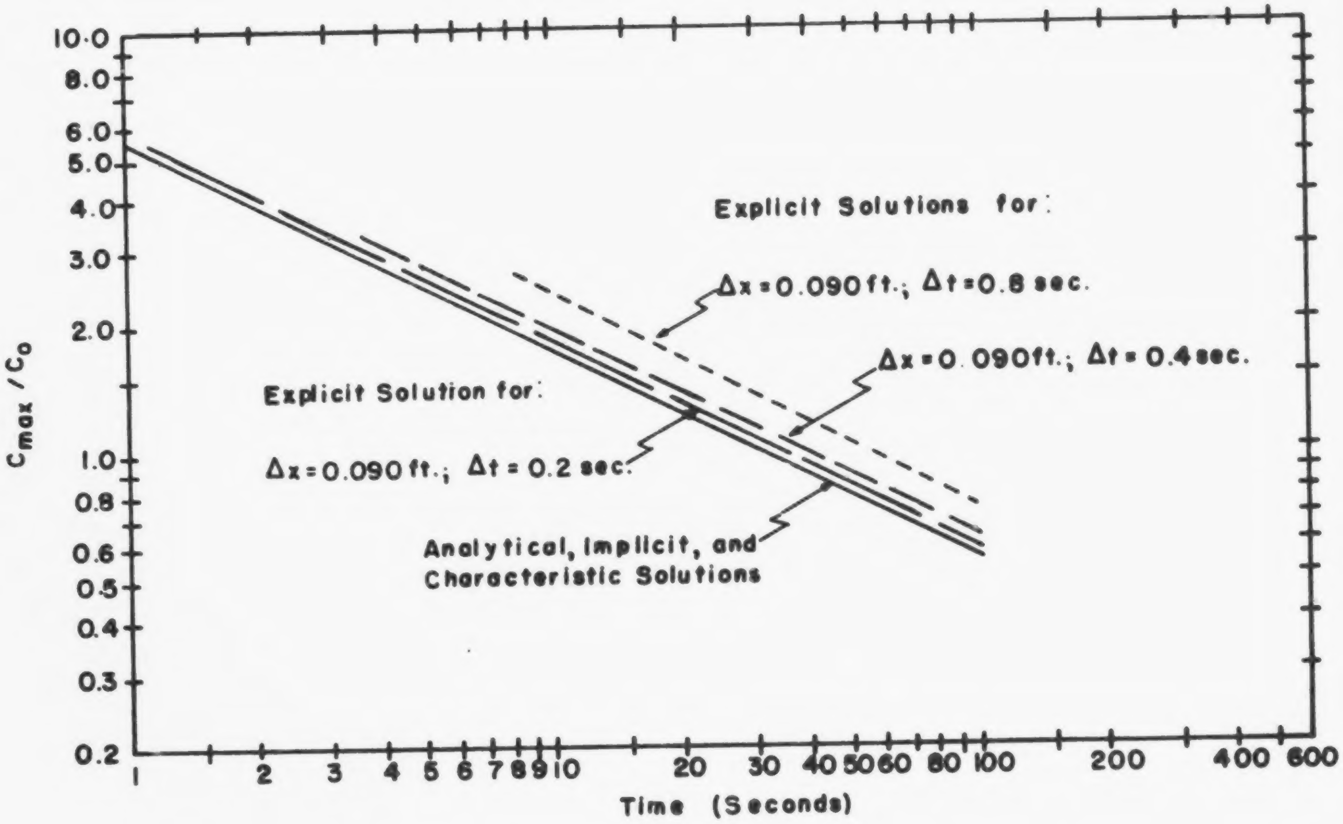

FIGURE 5-5 PLOT OF $C_{max.}/C_o$ VERSUS TIME FOR PLUG FLOW

The existence of errors with the stationary coordinate system of the explicit model prompted the search for a more accurate numerical method. The implicit model, as described in Chapter 4, was developed and tested on the plug flow problem. The results are shown in Figures (5. 3) and (5. 5) and are the same as the results of the explicit solution with the moving coordinate system and Equation (3. 8). As mentioned in the earlier discussion of the implicit model in Chapter 3, the incremental step sizes used in the implicit model were the same as those which met stability requirements in the explicit model; this insures an accurate approximation of $\frac{\partial c}{\partial t}$. With a larger number of calculations made in using the implicit method, it is extremely time consuming to use the implicit method for large grid systems.

The characteristic model when applied to the plug flow problem produced the same values for the dispersion coefficient as the implicit model. These results are also shown in Figures (5. 3) and (5. 5). The characteristic model had no restrictions on Δx, and Δt was restricted by Equation (3. 33). Several different sizes of Δx were used ranging from 0. 09 feet to 10 feet and the same correct results were always produced.

In summary, it should be noted that three procedures produced accurate solutions of the plug flow problem. They are the characteristic model, the implicit model, and the explicit model with the moving coordinate system. The explicit model with the stationary coordinate system did not produce an accurate solution for any data set, but when the dispersion coefficients of several solutions were compared, a graphical analysis produced an accurate solution. Even though the implicit model produced accurate solutions, the computation time was so great as to be considered a liability. The characteristic model was the most efficient, accurate model when solving the plug flow problems.

5-2 Shear Flow Test Problem

To test the general applicability of the computer models, a simple shear flow problem was hypothesized. The exact solution of the problem is unknown; therefore, the experience gained in processing the plug flow problem is to be used to interpret the results of the shear flow problem. In the shear flow problem, the lateral coefficient of turbulent diffusion is important in the dispersing of the diffusant. To simplify the problem, homogeneous isotropic turbulence is assumed, and therefore, the lateral coefficient of turbulent diffusion is the same as the longitudinal coefficient. As only a few grid points are to be used in the lateral direction, it would be presumptuous to make an interpretation of lateral dispersion. Consequently, the focus of the interpretations is directed to only longitudinal effects.

For the problem, values for each variable were selected which would be typical of the order of magnitude of the variable. The diffusion coefficients were selected to be 0.0025 square feet per second. A simple velocity distirbution was selected to be

$u(1) = 0.01$ fps

$u(2) = 0.02$ fps

$u(3) = 0.03$ fps

$u(4) = 0.02$ fps

$u(5) = 0.01$ fps (5.2)

The velocity distribution was arbitrarily chosen and has no physical relevance. As the plug flow problem had small increment sizes due to stability conditions when $E_x = 0.0025$ ft^2/sec, the maximum velocity for this problem was reduced so as to increase the step sizes. Undoubtedly, a velocity as low as 0.03 fps will decrease the difference between the diffusion coefficient and the computed dispersion coefficient. Nevertheless, the problem will provide insight into the applicability of the numerical methods.

The above data were processed several times in the explicit model. From Equations (3.32) and (3.33), the maximum values of the incremental steps are $\Delta x = 0.165$ feet and $\Delta t = 2.56$ seconds. The computer program then set a grid system where $\Delta x = \Delta y = 0.16$ feet. As the error inherent in the explicit method is proportional to Δx^2 and Δt, values of Δt were varied to check the accuracy of the solution. Values of the time increment were 2.5 seconds, 1.25 seconds, and 0.625 seconds. Unlike the plug flow problem where the calculated coefficient was constant, the calculated dispersion coefficient varies in the shear flow problem. Thus, the dispersion coefficient versus time was plotted on logarithmic graph paper, Figure (5.6).

Each of the three data sets were solved by the explicit method using both the moving and stationary coordinate systems. No differences

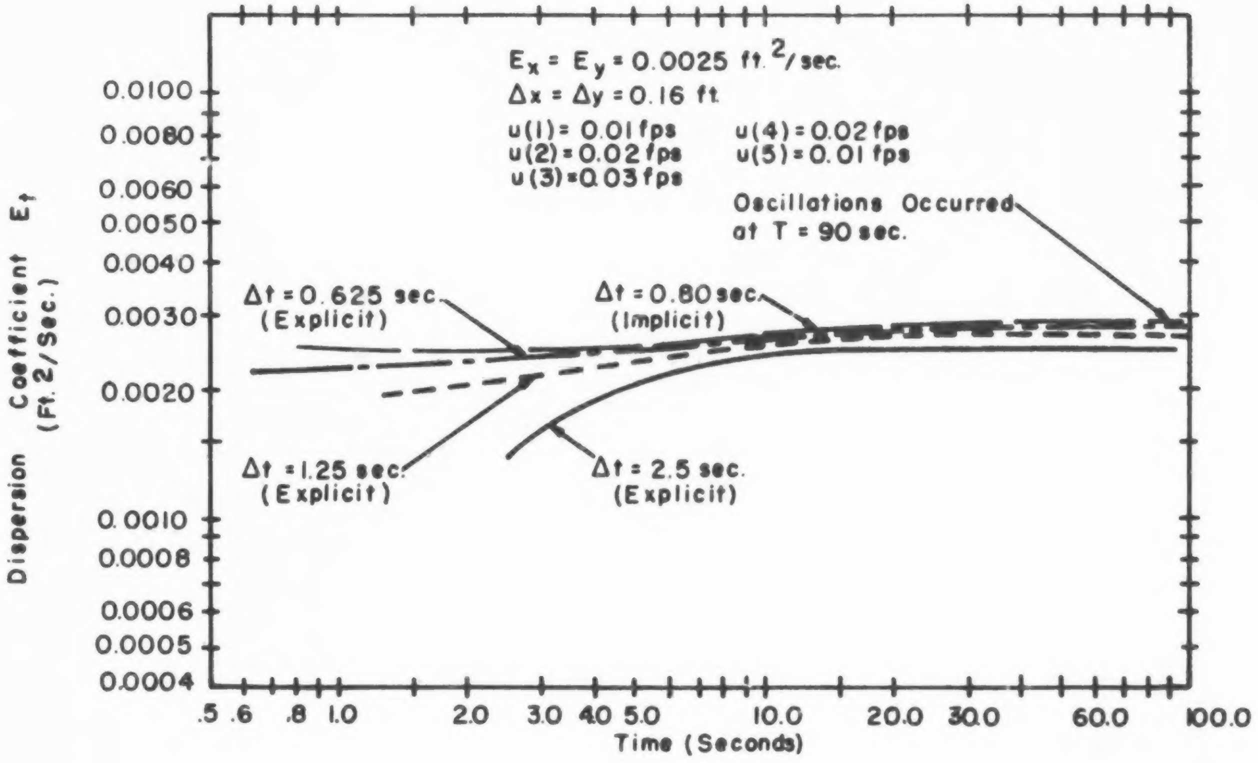

FIGURE 5-6 DISPERSION COEFFICIENT VERSUS TIME FOR SHEAR FLOW EXAMPLE PROBLEM

were detectable between the solutions obtained by use of either coordinate system. Thus, the solutions are reported simply as results of the explicit method. For each of the three data sets, the magnitude of the dispersion coefficient continued to increase with time until a constant value was attained. When the values of the dispersion coefficients for all data sets became constant as illustrated in Figure (5.6), their lines became parallel and offset from each other by constant values of long E_T. Plotting the constant value of the dispersion coefficient versus the temporal step size on arithmetic paper, Figure (5.7a), produced a straight line relationship similar to that of the plug flow problem. By projecting this line to $\Delta t = 0$ a value of the dispersion coefficient is attained where the effects of the error proportional to Δt are negligible. Processing a data set where $\Delta X = 0.08$ feet and $\Delta t = 2.5$ seconds produced the same solution as a data set where $\Delta X = 0.16$ feet and $\Delta t = 2.5$ seconds. Thus, the effects of any error proportional to $\overline{\Delta X}^2$ are negligible. Therefore, it can be concluded that as the effects of errors proportional to Δt and $\overline{\Delta X}^2$ are negligible, then the value of the dispersion coefficient projected to $\Delta t = 0$ on Figure (5.7a) may be assumed to be a correct solution.

As the solution for the dispersion coefficient yielded $E_T = 0.0029$ ft^2/sec and the input diffusion coefficient was $E_x = 0.0025$ ft^2/sec., then it is obvious that convective dispersion had little effect upon total dispersion in this problem. With convection producing little dispersion, longitudinal turbulent diffusion must have a greater role in total dispersion.

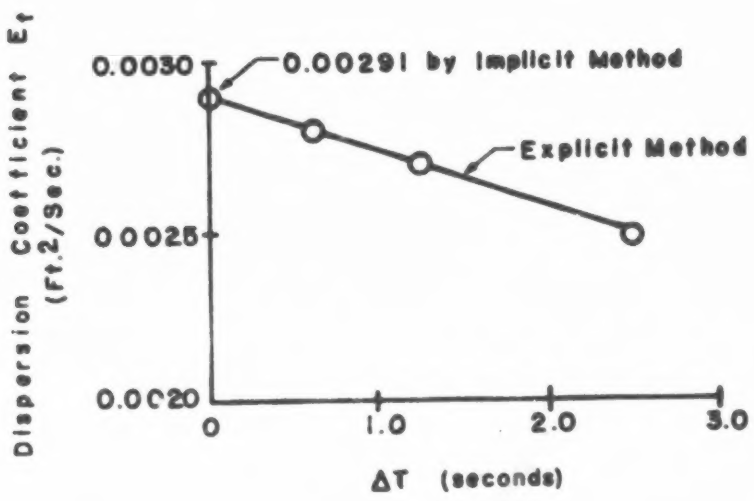

FIGURE 5-7a PLOT OF DISPERSION COEFFICIENT VERSUS STEP SIZE AT T = 100 sec.

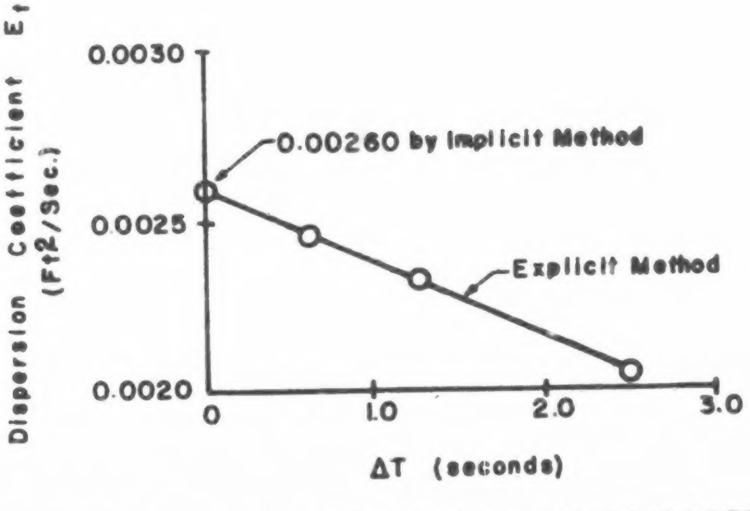

FIGURE 5-7b PLOT OF DISPERSION COEFFICIENT VERSUS STEP SIZE AT T = 05 sec.

The small role of convective effects in this problem is only because of the manner in which this problem was hypothesized.

When processing the above data with the implicit model, the same basic trend for growth of the dispersion coefficient with time was noted, Figure (5.6). The dispersion coefficient became constant and remained constant for many successive incremental steps. Suddenly, severe oscillations occurred in the concentration distribution which affected the magnitude of the dispersion coefficient and made the dispersion coefficient meaningless. The oscillations were traced to the errors introduced by incorrect longitudinal boundary conditions, refer to Chapter 4. In spite of the oscillations the constant value of the dispersion coefficient before the oscillations developed can be used for analytical interpretations. The value produced by the implicit method is greater than those produced by the explicit method and is equal in value to the result of the graphical analysis in Figure (5.7a). Producing the same value by two different techniques indicates that a reliable value of the dispersion coefficient has been obtained.

In viewing the data in Figure (5.6) before the constant value of dispersion coefficient is obtained, it is apparent that results of the intermediate computations approach the constant value asymptotically. Analyzing the dispersion coefficients at time equals 5 seconds and making an arithmetic plot of the values produced by the explicit model, Figure (5.7b), it is noted that again the same value of dispersion coefficient is produced by the implicit method and the projection of the explicit values back to Δt equals zero. Whenever sufficient experimental data becomes available, these methods may help to verify dispersion coefficients obtained before steady state conditions are reached.

Attempts to process the above data in the characteristic model met repeated failure. An analysis of the two conditions necessary for the applicability of the characteristic method,

$$\Delta x = u(y)\,\Delta t \qquad (3.51)$$

and

$$\Delta t < \frac{\overline{\Delta x}^2 \cdot \overline{\Delta y}^2}{2(E_x\,\overline{\Delta y}^2 + E_y\,\overline{\Delta x}^2)} \qquad (3.33)$$

shows that with the small values of Δy, E_x and E_y, no values of Δx and Δt can be obtained to meet both the stability requirement of Δt and the requirement that $u(y) \cdot \Delta t$ be a multiple of the grid increment Δx. Therefore, this shear flow problem cannot readily be solved by the characteristic model. Attempts were made to produce another hypothesized shear flow problem with different values of u, E_x and E_y; it was determined that no common shear flow problems exist which can be solved both explicitly, implicitly and characteristically. Primarily, no common problems exist because, the characteristic model as programmed works best for large values of u(y) and Δx, whereas, the explicit and implicit models require small values of Δx and Δt. Thus, a distinction exists between the types of problems which models can handle efficiently.

In summary it should be noted that the accuracy and efficiency of the explicit model is affected by the inclusion of convection. The explicit model produced accurate solutions only when results of several processings were subjected to graphical analysis. The implicit model produced accurate results until longitudinal boundary effects produced severe oscillations. No longitudinal boundary conditions could be contrived to eliminate these oscillations. The characteristic model could not work the problem because the increments were too small to meet necessary requirements. Perhaps the above statements are harsh, but they reflect an attitude of search for a method which can be universally applicable for all types of dispersion problems. If the search is only for a correct solution to the above problem, then methods have been shown to exist to obtain an accurate solution within reasonable limits.

5-3 Laboratory Stream Test Problem

To test the applicability of the models to naturally occurring phenomena, a problem was selected from the study of Fischer [1966a]. His data were gathered in a laboratory model of a stream with rough sides and a smooth bottom. A 40-meter flume with a flow width of approximately 36 cm was used to collect the data. The data are reported in Fischer's dissertation as series 2900. Fischer adopts the usage of the lateral diffusion coefficient determined by Elder [1959] and reports that no studies to date have conflicted with its statement of

$$E_y = 0.23\, du^* \qquad (5.3)$$

where d is the depth and u* is the shear velocity. As longitudinal turbulent diffusion is to be included in the problems of this study, and as one cannot accurately estimate the relationship between longtudinal and lateral turbulent diffusion coefficients, then the assumption of homogeneous, isotropic turbulence is made. Although homogeneous, isotropic turbulence probably did not exist in Fischer's study, there is no other basis on which to include longitudinal turbulent diffusion.

Fischer reports in his data on series 2900, a value of d=4.7 cm. and u*=3.59 cm/sec. Thus, by Equation (5.3) and the assumption of homogeneous isotropic turbulence, E_y and E_x equal 0.00417 square feet per second. Using 7 grid increments to represent the width of 36 cm, the value of Δy is 5 cm or 0.164 feet. Interpretations of the velocity distribution are given in Figure (5.8) with the maximum velocity being equal to 2.13 fps. The above data are the essential information required to use any computational algorithm.

Using the above information to determine the stability requirements for the explicit model, the maximum sized increments which can be used are $\Delta X = 0.0139$ feet and $\Delta t = 0.0201$ seconds. A computer run was tried with the explicit model. The explicit model was impractical because of the computer time necessary to perform the calculations for so many grid points. It required over 250 seconds of central processor time on a CDC 6600 computer to calculate 7.5 seconds of diffusion time, and this was on a grid which represented less than 10 feet of diffusion space. The main limitation was not on time but on storage capacity which was insufficient to construct the needed grid system. As the implicit method produces the best results when, the incremental steps meet explicit stability requirements, both the explicit and implicit methods were considered unsatisfactory to provide a practical solution to this problem.

The problem, being impractical for the explicit and implicit models, is more adaptable to the characteristic model. The characteristic model was used with both moving and stationary coordinate systems. If any variable representing a grid point in time and space is considered, then when comparing the value of the variable computed with the moving coordinate system to the value of the variable computed with the stationary coordinate system, there is absolutely no difference in the two values. Thus, the characteristic model is a major improvement over the explicit model.

The moving coordinate system is superior to the stationary system in that more efficient use is made of the grid system, because the moving coordinate system can be centered upon the centroid of the concentration distribution. Therefore, the following is a description of the necessary steps to implement the characteristic model with a moving coordinate system.

As previously mentioned in Chapters 3 and 4, some manipulation of the velocity distribution is necessary to fit the solution of the convection equation, Equation (3. 51), to the grid system. Thus, when concentration values are moved from one grid point to another by convection, the displacement will be a multiple of the grid increment ΔX. Figure (5. 8)

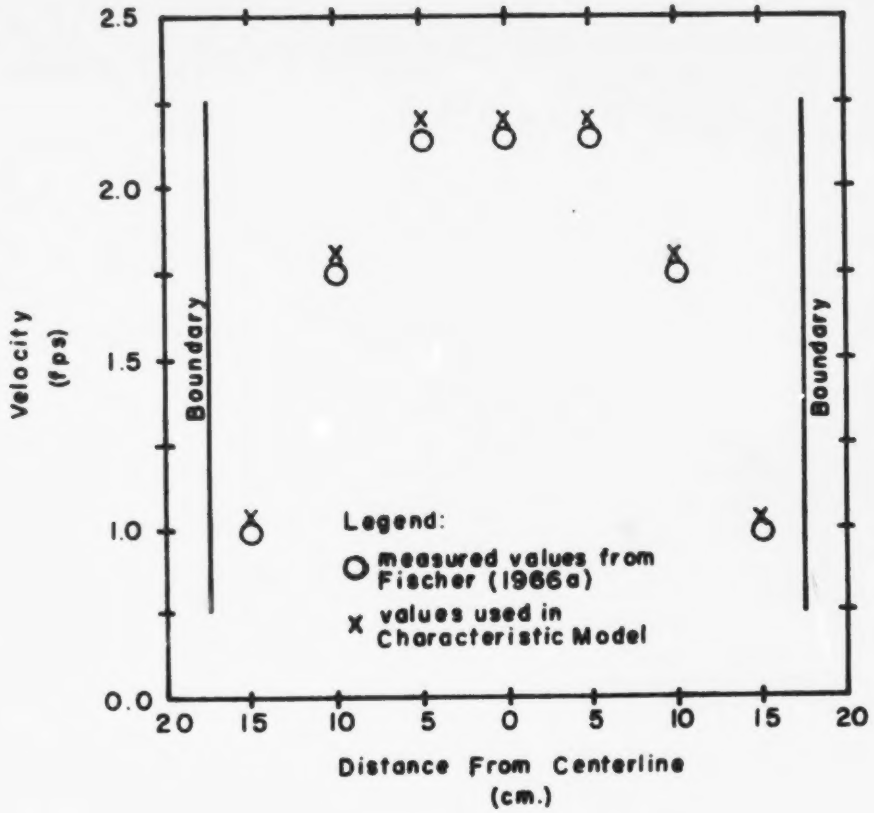

FIGURE 5-8 VELOCITY VALUES FROM FISCHER'S 2900 SERIES

shows the adjustments which were made to Fischer's velocity distribution. The maximum change in any velocity value was less than four percent. Using a velocity of 1.60 fps for the velocity of the coordinate system establishes a common multiple of 0.20 fps. The deviations from the velocity of the coordinate system are

$$
\begin{aligned}
u(1) &= -0.60 \text{ fps} \\
u(2) &= +0.20 \text{ fps} \\
u(3) &= +0.60 \text{ fps} \\
u(4) &= +0.60 \text{ fps} \\
u(5) &= +0.60 \text{ fps} \\
u(6) &= +0.20 \text{ fps} \\
u(7) &= -0.60 \text{ fps} \qquad (5.4)
\end{aligned}
$$

Thus, a system of velocities relative to a moving coordinate system is used to establish convective dispersion.

In checking stability conditions imposed by Equation (3.33), no value of ΔX could be found which would yield a range of Δt from values just meeting the stability criterion to those at one-fourth of stability. Thus, convergence could not be checked for a given value of ΔX. Since the magnitude of the error is proportional to $\overline{\Delta X}^2$ and to Δt, and if values of ΔX less than one are used, then the effects of errors proportional to $\overline{\Delta X}^2$ may be negligible. Thus, varying values of ΔX were used in the characteristic model. Values of Δt selected for a ΔX by Equation (3.33) were as close to stability conditions as possible. Selection of Δt values at stability conditions was made (1) to insure a large Δt and (2) to establish a uniform policy of selection. Values of ΔX which were used are 0.10, 0.25, 0.50 and 0.60 feet. The results of computer runs with the above data re presented in Figure (5.9). Oscillations are present during the early stages of computation, but they are dampened as the computations progress. Again, dispersion coefficients asymptotically approach a constant value.

Plotting the constant values of the dispersion coefficient versus temporal increment size, Figure (5.10), established a straight line relationship. This straight line appears to justify the assumption of a negligible magnitude of error proportional to $\overline{\Delta X}^2$. The linear relationship of Figure (5.10) indicates convergence to a dispersion coefficient of 1.975 square feet per second. Fischer [1966a], on the basis of several experimental and analytical determinations, reports a range of values for the dispersion coefficient of 2.71 to 3.85 square feet per second with a mean value of 3.17 square feet per second. The value determined by the characteristic model does not fall within the range reported by Fischer but is 38% less than the mean value, which is a reasonable correlation for many dispersion studies. Fischer reported and demonstrated that his range of mean concentration values with a ±15 percent variation was an excellent fit to the experimental data. Fischer's mean value of the total dispersion coefficient, 3.17 ft^2/sec, produced a maximum concentration, C_{max}/C_0, of 0.0224 in the equation for the solution of one dimensional convective diffusion, Equation (3.8). The value obtained by the above analysis, 1.975 ft^2/sec, produces a

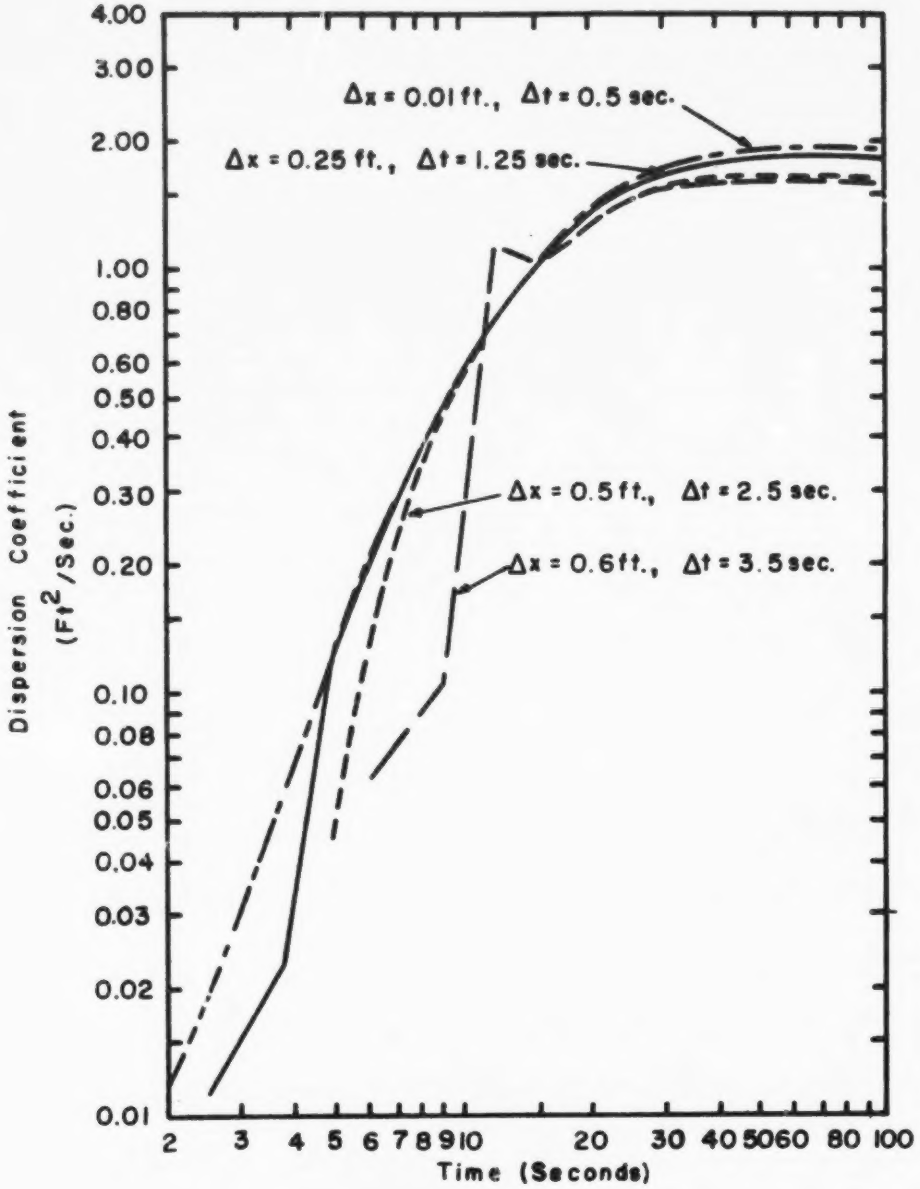

FIGURE 5-9 PLOT OF DISPERSION COEFFICIENT VERSUS TIME FOR FISCHER DATA

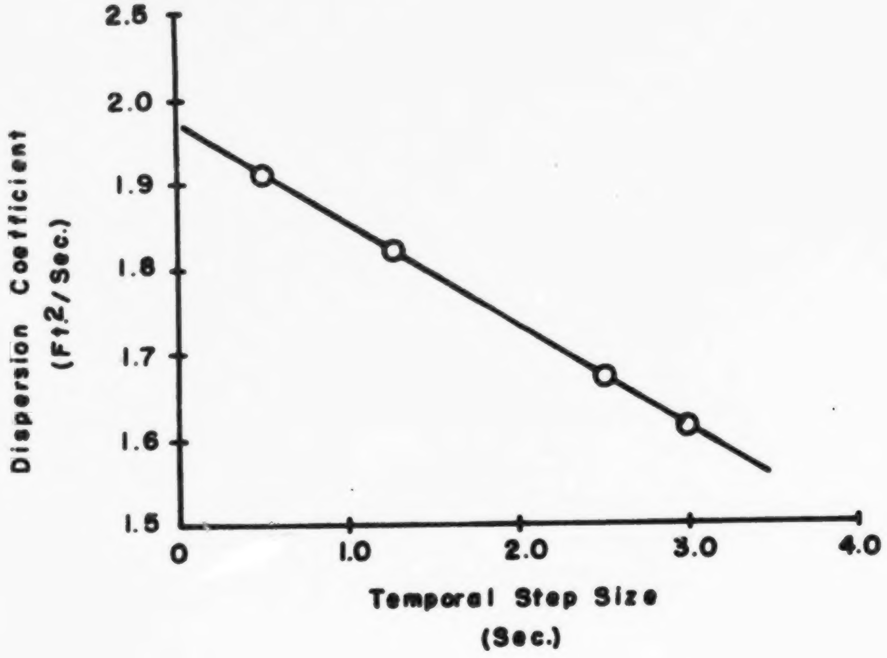

FIGURE 5-10 PLOT OF DISPERSION COEFFICIENT VERSUS TEMPORAL STEP SIZE FOR A LABORATORY STREAM

C_{max}/C_0 of 0.0284, a value 27 percent higher than that produced by Fischer's mean coefficient. Thus, the characteristic model has produced results which compare favorably with Fischer's investigation.

In summary, it has been demonstrated that the characteristic model produced adequate values of a dispersion coefficient for a problem which could not be solved by either the explicit or the implicit model. This was primarily due to the elimination of the restriction of ΔX. The ability of the characteristic model to adequately solve a naturally occurring problem by a numerically exact technique with a minimum of contrivance is a major improvement in solving convective dispersion problems. In addition, there was absolutely no difference in the values of any variable computed by either the moving coordinate system or the stationary coordinate system.

5-4 Two Dimensional Reservoir Test Problems

An attempt was made to apply the characteristic model to data gathered in Lake Austin. Lake Austin is a run-of-the-river reservoir located within the city limits of Austin, Texas. During the summer months the lake is stratified with the inflow to the lake becoming an undercurrent along the bottom of the lake and causing a circulation cell to exis above the thermocline. For the most part, the depth of the lake is between 15 and 20 feet. The conditions in Lake Austin are such that the lake can easily be regarded as a two dimensional lake; the two directional dimensions being longitudinal and vertical.

Figure (5.11) presents temperature and velocity profiles on a typical summer day for Lake Austin. To fit the velocity distribution to the characteristic model, the maximum deviation from the true velocity profile was 0.03 fps. The adjustments are also presented in Figure (5.11). A moving coordinate system was established with a velocity of 0.07 fps. The velocity deviations from the velocity of the coordinate system are

$$
\begin{aligned}
u(1) &= -0.28 \text{ fps} \\
u(2) &= -0.14 \text{ fps} \\
u(3) &= 0.0 \text{ fps} \\
u(4) &= +0.07 \text{ fps} \\
u(5) &= +0.14 \text{ fps} \\
u(6) &= +0.28 \text{ fps} \\
u(7) &= +0.21 \text{ fps} \\
u(8) &= +0.07 \text{ fps}
\end{aligned}
\qquad (5.5)
$$

This distribution has a common multiple of 0.07 fps.

The spatial increment in the vertical direction, Δy, was chosen to be 2.25 feet, thus, producing 8 vertical increments. As the magnitude of the velocities and the shear stresses in the lake were less than those in Fischer's laboratory stream, then the turbulence level was also less than that occurring in Fischer's stream. Consequently, values of the turbulent diffusion coefficients were chosen to be 0.0025 square feet per second. The above data were used to perform a stability check by Equation (3.33). For a value of $\Delta x = 1$ foot, a wide range of values

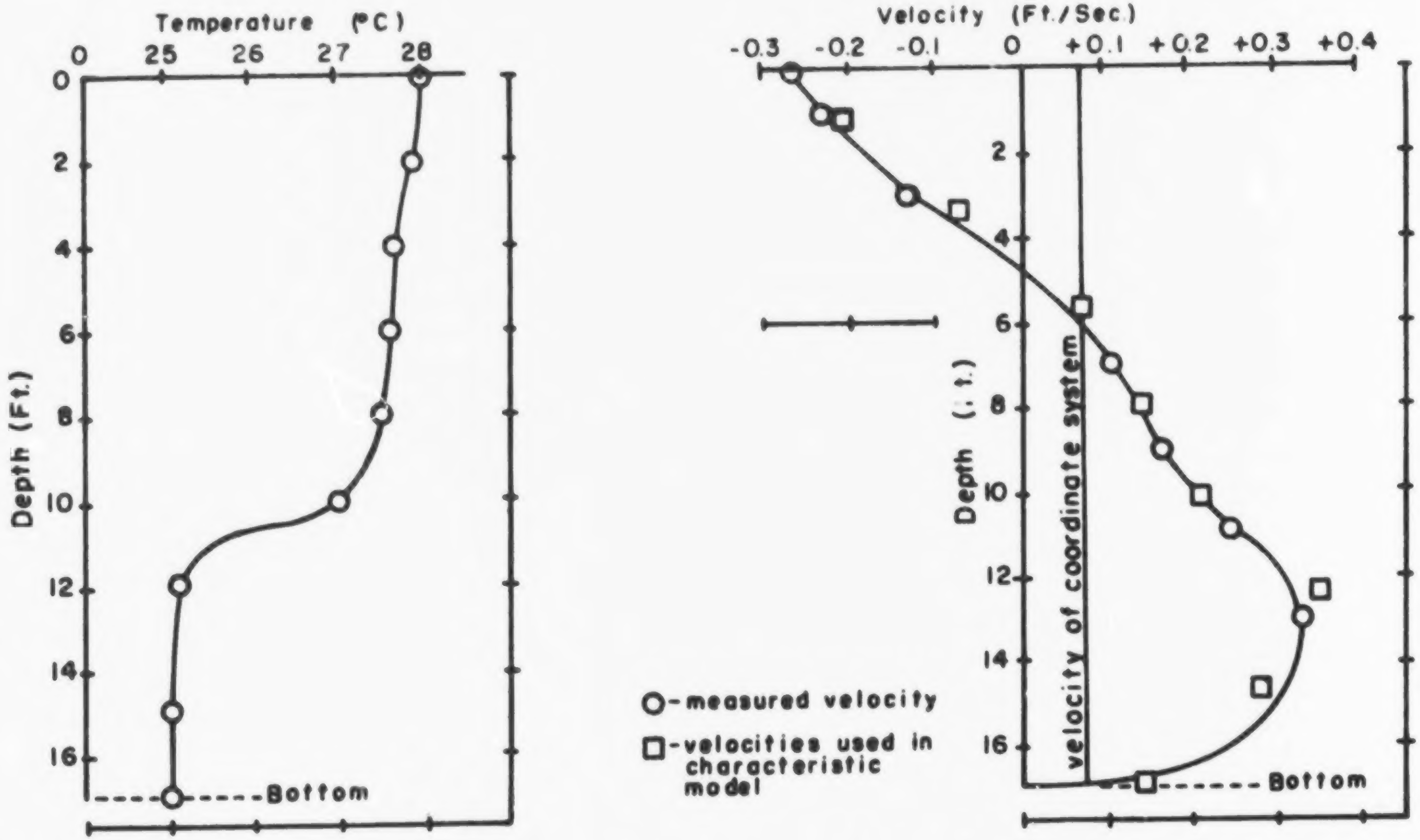

FIGURE 5-11 TEMPERATURE AND VELOCITY PROFILES OF LAKE AUSTIN, TEXAS ON AUGUST 19,1967

for Δt were available to meet both requirements for the characteristic model. Values of Δt equal to 71.429, 28.572 and 14.286 seconds were used to process the data for Lake Austin.

The results of the three data runs are presented in Figure (5.12). No constant values for the dispersion coefficients could be obtained. Instead the value of the dispersion coefficient continued to increase with time. The growth for all three processings of the data can be described by the relationship

$$E_T = t^{0.555} \tag{5.6}$$

The upper bound of this relationship is not known, but processing the data with a single run which occupied the entire storage of the CDC 6600 computer indicates that this relationship continues through 2500 seconds.

To expect that a constant dispersion coefficient would not occur during this time is reasonable. A constant dispersion coefficient occurs only when the dispersant is mixed to an approximately uniform concentration over the cross section. As the system is quite large and extensive and as the velocity distribution is irregular, then it is difficult for the diffusant to be uniformly mixed over the cross section. Even if the diffusant was uniformly mixed, its concentration value would be exceedingly small. In such a situation as occurs in this model of a lake, the movement and change in value of the maximum concentration is of primary concern. The characteristic model offers the technique by which such concerns can be studied.

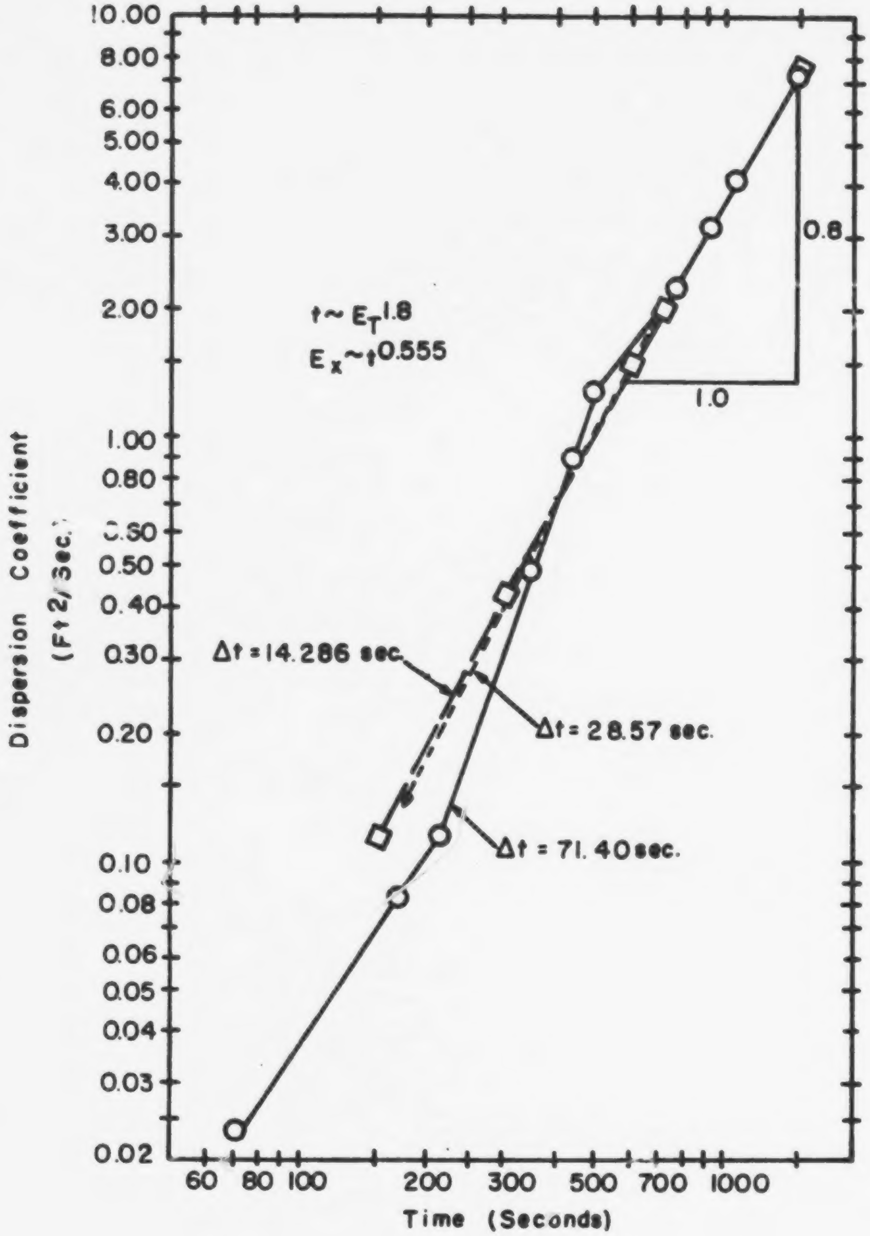

FIGURE 5-12 PLOT OF DISPERSION COEFFICIENT VERSUS TIME FOR LAKE AUSTIN DATE

In addition, the assumption that diffusant is injected uniformly over a cross sectional plane is unreasonable for a lake. Diffusant injection from either a line source or a point source would be a more reasonable assumption. In the two dimensional models which were constructed, dispersion from a line source could easily be determined. However, different techniques of reporting the dispersion coefficient and of handling the error analysis would have to be developed. To develop these techniques, suitable experimental data would be needed for proper verification. In order to study dispersion from point sources, a three dimensional characteristic model would have to be constructed, so that dispersion in three directions could be evaluated.

5-5 Summary of Computational Experience

The above problems provided a good test of all models, and from the above results several general statements can be made. The explicit model provided accurate results whenever convection was not included within the diffusion computations. Whenever convection was included with diffusion, accurate results were only produced whenever graphical analyses were made of the results of several computer processings. Also, whenever convection is included in the problem, the grid increment is severely restricted by

$$\Delta X < \frac{2E_x}{u} \qquad (3.32)$$

Thus, if the diffusion coefficient is small and u is large, then ΔX is unreasonably small. With ΔX being small, Δt is also small as its size is governed by Equation (3. 33). The problem utilizing Fischer's data is an excellent illustration of the severity of the above limitations. Nevertheless, the explicit method has produced satisfactory results whenever the relationship of E_x and u make the construction of an adequate grid feasible.

The implicit model is more accurate than the explicit model, but the implicit model is considerably more complicated and time consuming to apply. The best results are produced when the spatial and temporal step sizes meet the explicit stability conditions. Step sizes larger than those produce inaccurate approximations which can cause oscillations. In addition, the mathematical modeling of the longitudinal boundary conditions must be exactly accurate to prevent oscillations from developing in the results. The implicit method does not appear to have much future in the solution of the convective dispersion equation unless better mathematical representations of all boundary conditions can be developed.

The characteristic model was subjected to a broad spectrum of demands by the above problems. In the plug flow problem, the model demonstrated its accuracy. In the problem using Fischer's data, the model produced an adequate solution for a problem which could not be solved by either the explicit or implicit model. This means that some problems which could not be solved by exact numerical techniques can now be solved. Additionally, problems which fit into this category can be solved with a minimum of contrivance. A better approach to the problem of dispersion in a lake is by an analysis of dispersion from either line or point sources. The inability to use the characteristic model on the simple shear flow problem is attributable to limitations imposed by the construction of the characteristic model. If the characteristic method had been programmed in a manner similar to that of Garder, et al [1964], then the characteristic method could have also been used on the simple shear flow problem. The method by Garder, et al allows for the inclusion of low velocities by a dual grid system to approximate convection. The use of the dual grid system, however, does not allow for an exact integration of diffusion along characteristic lines as presented in Chapter 3. Consequently, it appears that the characteristic method cannot be programmed without some form of manipulation of the velocity distribution. The degree of manipulation of the velocity distribution for the characteristic method as programmed in this study or as programmed by Garder, et al is not excessive and does not appear to adversely affect the results.

5-6 Data Required for Use in Models

No model as developed was universally applicable to all two dimensional convective dispersion problems. However, all three of the models need the same basic information for input data.

First, the problem should be formulated for two dimensions. As the models have been restricted to one dimensional convection, the longitudinal axis, x, should be selected in the direction of flow. In those problems which are truly two dimensional, the selection of the second axis is obvious. For many naturally occurring problems, however, a choice for the second axis must be made between either the lateral or vertical direction. As a general rule, the second axis would be chosen in a direction corresponding to the channel dimension considered to be most representative of the scale of mixing within the cross section.

The temporally averaged velocity distribution for the two dimensional plane is the next essential item. The distribution can be obtained by direct measurement in the field or laboratory. When the velocity profile is a frequently observed distribution such as in the case of the "universal" velocity distribution in a pipe, then theoretical analysis can yield the desired velocity profile. Whether the velocity distribution is obtained by direct field measurement or by theoretical analysis, it is the most essential input item for a model.

The coefficients of turbulent diffusion, E_x and E_y should next be determined. As Taylor [1954] demonstrated, the effects of convective displacement are two hundred times greater than the effects of longitudinal turbulent diffusion for flow in pipes. Whenever a physical situation occurs such that the dispersive effects of turbulent diffusion are small relative to the dispersive effects of convection, the value of the turbulent diffusion coefficient becomes less important. Often, an order of magnitude for the turbulent diffusion coefficient can be estimated. In such cases, the extreme values covering the range can be processed separately in the model. If there is little change in the results of the total dispersion coefficient, then any value within that range may be used. If there is significant change in the results, then appropriate steps should be taken to determine the exact value of the turbulent diffusion coefficient.

Chapter 6

SUMMARY, CONCLUSIONS AND RECOMMENDATIONS

6-1 Summary

The solution of the convective dispersion equation is important when describing the concentration distributions which result when material is injected into a shear flow. When making reference to diffusion and dispersion, diffusion refers to the phenomenon of pure molecular diffusion or pure turbulent diffusion, and dispersion refers to convective displacement or any combination of convective displacement and diffusion.

Approximate solutions to dispersion may be obtained by using dispersion coefficients in the analytical solution of the one dimensional convective diffusion equation. The dispersion coefficient is determined by integrating the variations of the velocity distribution and lateral diffusion over the cross section. Useful dispersion coefficients have been determined by Taylor [1954] for pipe flow, Fischer [1966a and 1967] for open channel flow and Bowden [1965] for estuaries and the sea.

The numerical integration of the convective dispersion equation produces a numerical replica of a concentration distribution. A dispersion coefficient to characterize the distribution can be computed. Thus,numerical integration produces the same basic results which

Taylor, Fischer and Bowden performed analytically. The advantage of numerical integration over analytical integration is the inclusion of temporal effects which affect the early stages of dispersion and the possibility of including time dependent variations of velocity and turbulent diffusion coefficients. Three methods for numerical integration exist; they are the explicit method, the implicit method and the characteristic method. These three methods provide a generality to numerical methods which permit application to a broad range of problems.

6-2 Conclusions

Based upon the results of the preceding study, the following evaluations can be made for each numerical method. The evaluations are only for numerical solutions to the two dimensional convective dispersion equation,

$$\frac{\partial c}{\partial x} = E_x \frac{\partial^2 c}{\partial x^2} + E_y \frac{\partial^2 c}{\partial y^2} - u(y) \frac{\partial c}{\partial x}. \qquad (2.14)$$

(a) The method of characteristics is capable of solving problems which cannot be solved by either explicit or implicit techniques. The characteristic method can handle best those problems which have large velocities and small turbulent diffusion coefficients. This category fits most naturally occurring problems. The method of characteristics eliminates the constraint on the longitudinal spatial increment, ΔX. Additionally, the characteristic method has been verified to be accurate for both moving and stationary coordinate systems.

(b) The explicit method is accurate under plug flow conditions, but the spatial and temporal step increments are severely restricted for low values of dispersion coefficients, a result similar to that reported by Harleman, et al [1968]. Shear flows have increments which are even more restrictive.

Additionally, whenever convection terms are included within the model, a "pseudo" dispersion occurs. Nevertheless, under proper conditions the explicit method is easy to apply and is accurate within limitations.

(c) The implicit method is more accurate than the explicit method, but is more difficult to apply to problems. For plug flow conditions, the method is accurate. For shear flow conditions, the implicit method is accurate until oscillations develop. The oscillations are produced by incorrect assumptions of the longitudinal boundaries. Incremental step sizes with the implicit method should be restricted to values which meet the stability conditions of the explicit method.

(d) This study indicates that the mathematical representation and interpretation of all boundary conditions is an extremely critical phase of all methods, especially in the implicit method.

It should be noted that no method as developed is universally applicable for all two dimensional dispersion problems. The choice of the model to use on any given problem should depend upon the nature of problem and the magnitudes of the variables.

6-3 Recommendations

Based on the results of this study, the following recommendations for future research are made:

(a) The mathematical representation and interpretation of all boundary conditions should be given more attention. Proper representation of boundary conditions is extremely critical for the implicit methods.

(b) The search for a universally applicable model for all two dimensional convective dispersion problems should be continued by programming the method of characteristics in the manner of Garder, et al [1964]. Their method allows for two grid systems, one for convection and one for diffusion. If their procedure is followed, restrictions on the size of ΔX should be eliminated. In this study, no evaluation of the characteristic method could be made for problems with low valued turbulent diffusion coefficients.

(c) A three dimensional model should be constructed. With the method of characteristics, the construction of a model for three spatial dimensions is now feasible for large computers. Problems that do not fit the two dimensional simplification could then be solved.

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TABLE A-1

NOTATION AND CONVERSION EXPLICIT MODEL - PROGRAM DIFFU

Input Parameters

FORTRAN Notation	General Notation	Description
DX, DY	E_x, E_y	Turbulent Diffusion Coefficients (ft^2/sec).
X	Δx	Spatial Increment (feet).
T	Δt	Temporal Increment (seconds).
TI, TP		Printing Time Increment (seconds).
TL		Total Time for Dispersion (seconds).
LX, LY, LT	I,J,K	Number of Grid Points
LPS		Type of Diffusant Injection Source (Positive Number for Plane Source; Zero for Line Source).
KCX, KCY		Grid Point Location of Diffusant Injection Source.
UD(LY)	u(y)	Velocity Profile over Cross Section (fps).

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Internal Parameters

TT		Total Time Processed.
CHEKX		Maximum Permissible Value of Δx
CHEKT		Maximum Permissible Value of Δt
XDI(LX)		Longitudinal Position of LX with Respect to Dispersant Input.
SD	σ_t	Standard Deviation.
SK		Skewness.
PK		Peakedness.
EX	E_T	Dispersion Coefficient.
PREC	P. I.	Precision Index.
CM	C_{max}	Maximum Concentration.
XMC		Location of CM.
CPER		Cumulative Percent of Concentration Starting from LX=1.
C		Total Concentration in Element of Area $\Delta x \cdot \Delta y$
P	C	Concentration in Mass per Unit Area.

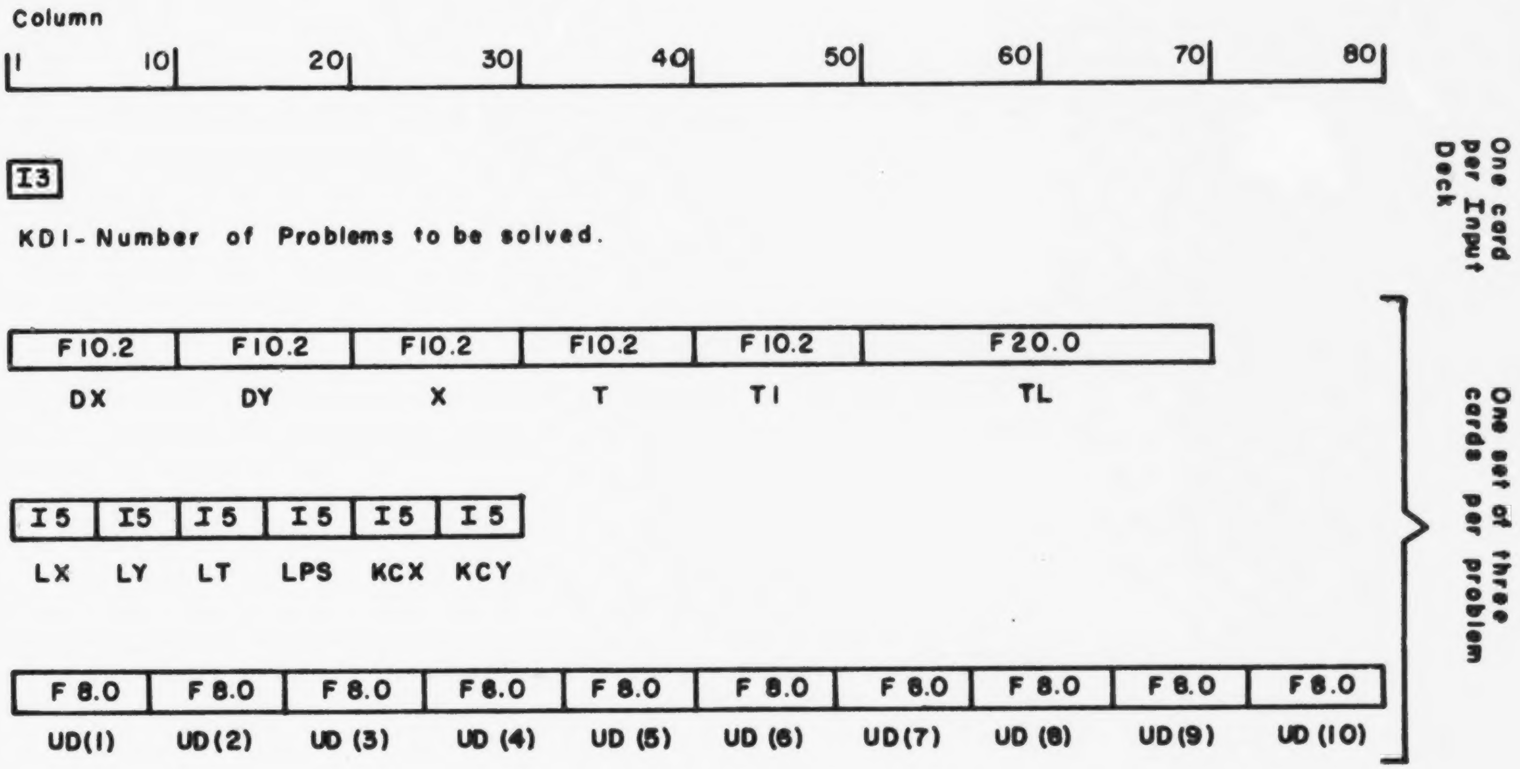

FIGURE A-1

GUIDE FOR DATA INPUT,
EXPLICIT MODEL PROGRAM DIFFUI

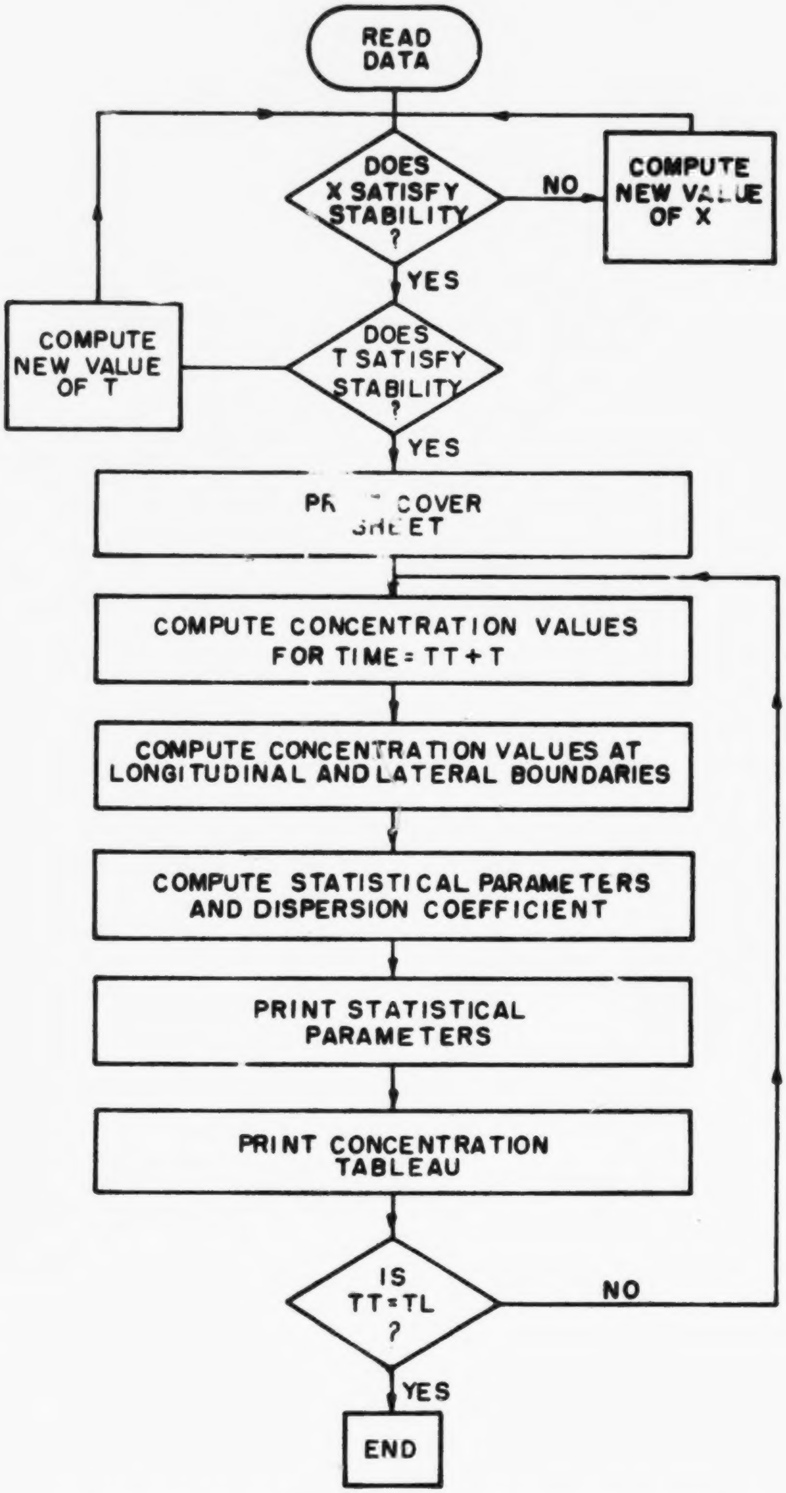
READ DATA
DOES X SATISFY STABILITY ?
NO
COMPUTE NEW VALUE OF X
YES
DOES T SATISFY STABILITY ?
COMPUTE NEW VALUE OF T
YES
PRINT COVER SHEET
COMPUTE CONCENTRATION VALUES FOR TIME = TT + T
COMPUTE CONCENTRATION VALUES AT LONGITUDINAL AND LATERAL BOUNDARIES
COMPUTE STATISTICAL PARAMETERS AND DISPERSION COEFFICIENT
PRINT STATISTICAL PARAMETERS
PRINT CONCENTRATION TABLEAU
IS TT = TL ?
NO
YES
END

FIGURE A-2 FLOW CHART FOR EXPLICIT MODEL

```
      PROGRAM DIFFU(INPUT,OUTPUT)
      DIMENSION C(120,10,10) ,UD(10), P(120,10), CPER(120, 1), XDI(120),
     1 PREC(10),FX(10),XMC(10),CM(10),VXP(10),SD(10),SK(10),PK(10)
  100 FORMAT (8H CHEKX = , F15.5, 10X, 5HX WAS , F15.7)
  101 FORMAT (8H CHEKT = , F15.5, 10X, 5HT WAS , F15.7)
  102 FORMAT (6I5)
  104 FORMAT (5F10.2,F20.0)
  105 FORMAT (I3)
  106 FORMAT (1H1)
  107 FORMAT (40X, 13H GRID SIZE IS, F7.4, 8H FEET BY, F7.4, 5H FEET,
     1 10X, 8H TIME IS,F17.4, 4H SEC/ 20X,31HCENTROID OF DISTRIBUTION IS
     2 AT ,F13.3, 30H FEET   STANDARD DEVIATION IS ,F13.5,5H FEET/1H1)
  108 FORMAT (10F8.0)
  109 FORMAT (17H FAILURE ON ITERM)
  110 FORMAT (5X,I4,5F15.10,5X,F15.8 ,F13.3)
  111 FORMAT (////,50X,15HSUMMARY OF DATA,//,40X,17HGRID INCREMENT IS,
     1F7.4,8H FEET BY,F7.4,5H FEET,/,40X,17HTIME INCREMENT IS,F10.4,9H
     2SECONDS,/,40X,23HTOTAL TIME PROCESSED IS,F17.4,9H  SECONDS,//,40X,
     330HCOEFFICIENTS OF EDDY VISCOSITY,/,50X,5HDX = ,F10.4,23H SQUARE F
     4FET PER SECOND,/,50X,5HDY = ,F10.4,23H SQUARE FEET PER SECOND,//
     5        //,40X,22HSTABILITY REQUIREMENTS,/,50X,19HMAXIMUM DISTANCE
     6 IS,F10.4,5H FEET,/,48X,19H  MAXIMUM TIME IS  ,F12.4,8H SECONDS,//
     7,60X,16HVELOCITY PROFILE,/,50X,5HPOINT,15X,17HVELOCITY (FT/SEC),//
     8(50X,I3,17X,F10.4,/))
  113 FORMAT (1H+,  9X, 1HR, 37X, 1HC, 36X, 1HR)
  114 FORMAT (10X, 1H1, 37X, 1H1, 36X, 1H1.  6X, 13HCUMU PCT CONC , 4X,
 1141 8HDISTANCE )
  116 FORMAT(1H1////33X,58HMATERIAL INTRODUCED AS AN INSTANTANEOUS LINE
     1SOURCE AT X =  ,I3)
  117 FORMAT(1H1////34X,57HMATERIAL INTRODUCED AS AN INSTANTANEOUS POINT
     1 SOURCE AT ( ,I3,1H,,I2,1H))
  118 FORMAT(1H1,12X,4HTIME,14X,3HU*T,13X,6HX MEAN,10X,7HSTD DEV,9X,
     1    9HDISP COEF )
  119 FORMAT (//3X,4HTIME,3X,4HITER,3X,7HY POINT,2X,8HMAX CONC,3X,
     18HCENTROID,4X,8HSTAN DEV,5X,8HSKEWNESS,3X,10HPEAKEDNESS,3X,
     29HPRECISION,4X,16HDISPERSION COEFF/ 4X,3HSEC,21X,4HC/CI,8X,2HFT,
     310X,2HFT,34X,5HINDEX,9X,9HFT**2/SEC / F9.2,I4,5X,I3,F13.5,F12.4,
     43F12.5,F13.5,F19.10/(18X,I3,F13.5,F12.4,3F12.5,F13.5,F19.10))
  120 FORMAT(25H MAXIMUM CONCENTRATION AT,F10.4,12H SECONDS IS ,F15.10)
C
C                               DEFINITIONS FOR INPUT DATA
C                  KD1        THE NUMBER OF PROBLEMS TO BE SOLVED
C                  DX         DIFFUSION COEFFICIENT, X DIRECTION
C                  DY         DIFFUSION COEFFICIENT, Y DIRECTION
C                  X          GRID INCREMENT (FEET)
C                  T          TIME INCREMENT (SECONDS)
C                  TI         PRINTING TIME INCREMENT (SECONDS)
C                  TL         TIME AT END OF PROBLEM (SECONDS)
C                  LX         NUMBER OF GRID POINTS, X DIRECTION
C                  LY         NUMBER OF GRID POINTS, Y DIRECTION
C                  LT         NUMBER OF GRID POINTS, T DIRECTION
C                  LPS        EITHER LINE SOURCE (ZERO) OR PLANE SOURCE (ANY
C                               POSITIVE NUMBER)
C                  KCX        LOCATION OF DYE INSERTION, X DIRECTION
C                  KCY        LOCATION OF DYE INSERTION, Y DIRECTION
C                  UD         ARRAY OF MEAN VELOCITIES IN THE X DIRECTION
C
      TS=0.0000000001  $  TSS=TS*100.
      READ 105, KD1    $   DO 18 KD2=1,KD1
C         DATA READ IN
      READ 104, DX,DY,X,T,TI,TL    $   READ 102, LX,LY,LT,LPS,KCX,KCY
      READ 108, (UD(K),K=1,LY)  $  U=ABSF(UD(1))  $  DO 42 K=2,LY
      IF (ABSF(UD(K)).GT.U) 43,42
   43 U = ABSF(UD(K))
   42 CONTINUE
      DO 1 IY=1,LY   $   VXP(IY)=0.   $   DO 1 IX=1,LX
    1 C(IX,IY, 1)=0.0 $ Y=X $ ITER=TT=EXP=0. $ ITERM=10 $ TP=TI
    9 ITER=ITER+1   $   IF (ITER.GE.ITERM) 98,6
   98 PRINT 109   $   GO TO 18
C         CHECK FOR STABILITY OF X INCREMENT AND CORRECTION IF NECESSARY
    6 IF(U)36,37
   36 CHEKX=2*DX/U $ GO TO 38
   37 CHEKX=  X  $ GO TO 38
   38 V=1.0 $ IF(CHEKX.GE.X)10,7
    7 PRINT 100, CHEKX, X   $   LAX=CHEKX   $   IF (CHEKX.LT.1.0) 23,24
   23 V=V*10   $   LAX=V*CHEKX   $   IF (LAX.GE.1) 24,25
   24 X=Y=LAX/V   $   GO TO 9
C         CHECK FOR STABILITY OF TIME INCREMENT AND CORRECTION, IF
C         NECESSARY
   10 CHEKT=(X*Y)**2/2/(DX*Y*Y+DY*X*X)   $   V=1.0
      IF (CHEKT.GE.T) 14,11
   11 PRINT 101, CHEKT, T   $   LAX=CHEKT   $   IF (CHEKT.LT.1.0) 2,3
    2 V=V*10   $   LAX=V*CHEKT   $   IF (LAX.GE.1) 3,2
    3 T=LAX/V   $   GO TO 9
   14 LTM1=LT-1   $   LYM1=LY-1   $   LXM1=LX-1 $  LYM2=LY-2
      IF (IPS.EQ.0) 60,61
   60 PRINT 116, KCX   $   DO 12 KK=1,LY
   12 C(KCX,KK,1)=1.0   $   AREA=X   $  GO TO 62
C         PRINTING OF COVER SHEET
   61 PRINT 117, KCX, KCY   $   C(KCX,KCY,1)=1.0   $   AREA = X*Y
   62 PRINT 111, X,Y,T,TL,DX,DY,CHEKX,CHEKT,((I,UD(I+1)),I=1,LYM2)
      PRINT 106  $  XDI(1)=(KCX-1)*(-X)  $  DO 63 KX=2,LX
   63 XDI(KX)=XDI(KX-1)+X
      CX=DX*T/X**2   $   CY=DY*T/Y**2     $  TT=TS
   44 DO 39 IT=1,LTM1  $  DO 16 IY=2,LYM1
C         COMPUTATION OF CONCENTRATION VALUES
      U=UD(IY)  $  CU=U*T/2./X  $  DO 16 IX=2,LXM1
      C(IX,IY,IT+1)=C(IX,IY,IT)*(1.-2.*CX-2.*CY) + C(IX+1,IY,IT)*
     1(CX-CU) + C(IX-1,IY,IT)*(CX+CU) + C(IX,IY+1,IT)*CY
     2 + C(IX,IY-1,IT)*CY
      IF (IY.EQ.LYM1) 25,26
C         COMPUTATION OF LATERAL BOUNDARY CONDITIONS
   25 C(IX,1,IT+1)=C(IX,2,IT+1)   $   C(IX,LY,IT+1)=C(IX,LYM1,IT+1)
   26 IF (IX.EQ.LXM1) 27,16
   27 C(1,IY,IT+1) = C(LX,IY,IT+1) = 0.0
C         COMPUTATION OF LONGITUDINAL BOUNDARY CONDITIONS
      IF((C(IX, IY,IT+1).GE.TS) .AND. (C(2, IY,IT+1).GE.TS))29,33
   33 IF((C(IX, IY,IT+1).LT.TS) .AND. (C(2, IY,IT+1).LT.TS))16,34
   34 LM=2   $   IF (C(IX, IY,IT+1).GT.TS) 31,32
   29 DO 28 LM=1,2   $   IF (LM.EQ.1) 31,32
   32 K1=1   $   K2=2   $   K3=3   $   K4=4   $   K5=5   $   GO TO 30
   31 K1=LX  $  K2=LX-1  $  K3=LX-2  $  K4=LX-3  $  K5=LX-4
   30 DC1=C(K3, IY,IT+1)/C(K2, IY,IT+1)
      DC2=C(K4, IY,IT+1)/C(K3, IY,IT+1)
      DC3=C(K5, IY,IT+1)/C(K4, IY,IT+1)
      DC=ABSF(DC1-DC2)+ABSF(DC2-DC3)+DC1
      C(K1, IY,IT+1)=C(K2, IY,IT+1)/DC
   28 CONTINUE
   16 CONTINUE  $  TT=TT+T  $  DO 53 M=2,LYM1  $  VX=SX=PX=XMC(M)=J=N=0.
C         COMPLETION OF CONCENTRATION CALCULATIONS. START CALCULATION OF
C         DISPERSIVE PARAMETERS
      DO 50 KX=1,LX   $   IF (C(KX,M,IT+1).GT.TS) 49,50
   49 XMC(M)=XMC(M)+XDI(KX)*C(KX,M,IT+1)   $   J=J+1   $   JA=KX
   50 CONTINUE  $  JB=JA-J  $  DO 52 KX=JB,JA   $ XST=XDI(KX)-XMC(M)
      TE=XST*C(KX,M,IT+1) $ VX=VX+XST*TE  $  SX=SX+TE*XST**2 $ IF(N)52,54
   54 CM(M)=0.   $   IF (ABSF(XST).LT.TEST) 51,52
   51 CM(M)=C(KX,M,IT+1)/AREA  $   N=1
   52 PX=PX+TE*XST**3 $ SD(M)=SQRTF(VX) $ SK(M)=SX/SD(M)**3
      PK(M)=PX/SD(M)**4 $ FX(M)=(VX  - VXP(M))/2./T $ VXP(M)=VX
   53 PREC(M)=3.*SK(M)**2-2.*PK(M)+6.
C         PRINTING OF STATISTICAL PARAMETERS.
C                CM = MAXIMUM CONCENTRATION
C               XMC = LOCATION OF CM
C                SD = STANDARD DEVIATION
C                SK = SKEWNESS
C                PK = PEAKEDNESS
C              PREC = PRECISION INDEX
C                FX = DISPERSION COEFFICIENT
      PRINT 119, TT,ITER,(IY,CM(IY),XMC(IY),SD(IY),SK(IY),PK(IY),
     1   PREC(IY),FX(IY), IY=2,LYM1)
      IS=1  $  IF (TT.LT.TL) 40,5
   40 IS=0 $ IF (TT.GE.TP)5,39
    5 CSUM=0.0  $  PRINT 106
      DO 45 KX=1,LX  $  CSUM=CSUM+C(KX, 3,IT+1)  $  DO 45 KY=1,LY
   45 P(KX,KY) = C(KX,KY,IT+1)/AREA $KY=3 $  CSUM=2.*CSUM
      CPER(1,1)=C(1,KY,IT+1)/CSUM*100.  $  DO 46 KX=2,LX
   46 CPER(KX, 1)=(C(KX,KY,IT+1) +C(KX-1,KY,IT+1))/CSUM*100.+CPER(KX-1,
     11)
      PRINT 113 $ PRINT 114  $  KT=IT+1
C        PRINTING OF CONCENTRATION TABLEAU
      PRINT 110, (KX,(P(KX,KY),KY=2,LYM1),CPER(KX, 1),XDI(KX),KX=1,LX)
      PRINT 107,X,Y,TT,XMC(3),SD(3)  $  TP=TP+10.   $  IF(LS)18,39
   39 CONTINUE $ DO 41 IX=1,LX  $  DO 41 IY=1,LY
C        WHEN LT TIME INCREMENTS HAVE BEEN PROCESSED, RETURN TO LT = 1
   41 C(IX,IY,1) = C(IX,IY,LT)  $ GO TO 44
   18 CONTINUE
      END
```

TABLE B-1

NOTATION AND CONVERSION IMPLICIT MODEL - PROGRAM DIFFUI

Input Parameters

FORTRAN Notation	General Notation	Description
DX, DY	E_x, Ey	Turbulent Diffusion Coefficients (ft^2/sec).
X	Δx	Spatial Increment (feet).
T	Δt	Temporal Increment (seconds).
TI, TP		Printing Time Increment (seconds).
TL		Total Time for Dispersion (seconds).
LX, LY, LT	I,J,K	Number of Grid Points.
IFPTSC		Type of Diffusant Injection Source (Positive Number for Plane Source; zero for Line Source).
KCX, KCY		Grid Point Location of Tracer Injection Source.
UD(LY)	u(y)	Velocity Profile over Cross Section (fps).

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Internal Parameters

TT		Total Time Processed.
XDI(LX)		Longitudinal Position of LX with Respect to Dispersant Input Condition.
SD	σ_t	Standard Deviation.
PK		Peakedness.
SK		Skewness.
EX	E_T	Dispersion Coefficient.
PREC	P. I.	Precision Index
CM	C_{max}	Maximum Concentration.
XMC		Location of CM.
CPER		Cumulative Percent of Concentration from LX=1.
C, CY		Total Concentration in Element of Area
P	C	Concentration in Mass per Unit Area.
CX	C^*	Concentration Value for Mid-step.
BXP1, BXM1, BY, GAM, GAMY, GAMT, ALPH, PSIX, PSIY		Simplification Terms for Commonly Occurring Relationships in Equations (3. 37), (3. 38) and (3. 39).

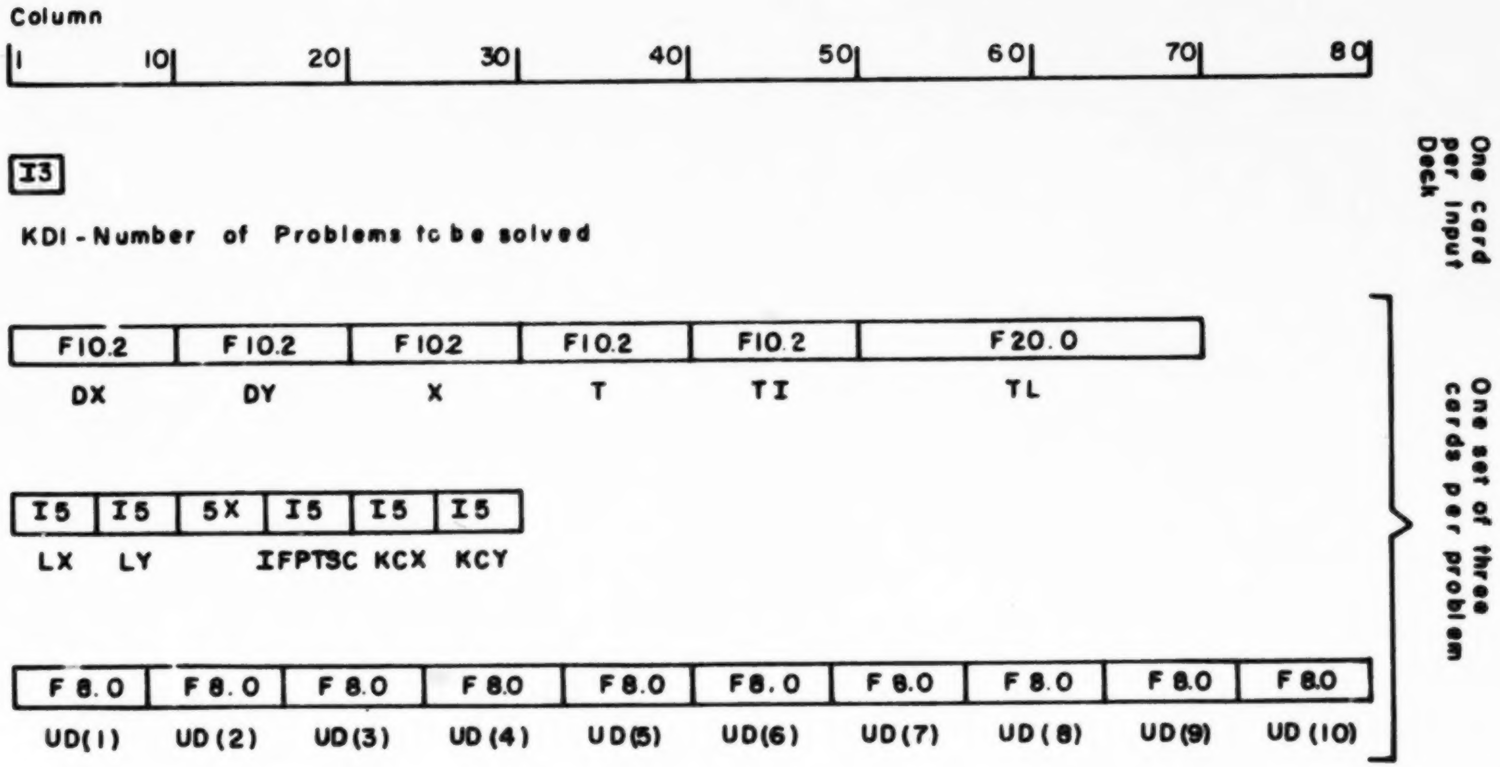

FIGURE B-1

GUIDE FOR DATA INPUT,
IMPLICIT MODEL-PROGRAM DIFFUI

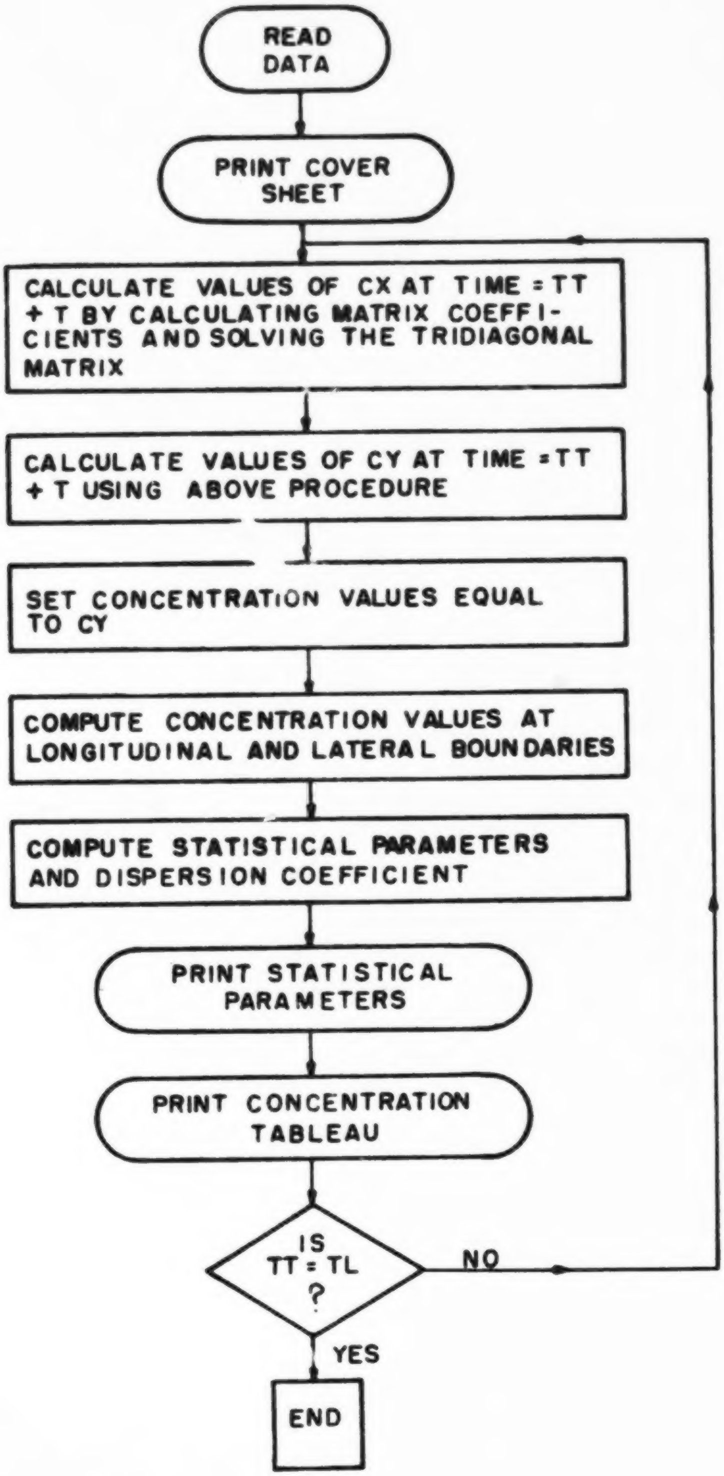
READ DATA
PRINT COVER SHEET
CALCULATE VALUES OF CX AT TIME = TT + T BY CALCULATING MATRIX COEFFICIENTS AND SOLVING THE TRIDIAGONAL MATRIX
CALCULATE VALUES OF CY AT TIME = TT + T USING ABOVE PROCEDURE
SET CONCENTRATION VALUES EQUAL TO CY
COMPUTE CONCENTRATION VALUES AT LONGITUDINAL AND LATERAL BOUNDARIES
COMPUTE STATISTICAL PARAMETERS AND DISPERSION COEFFICIENT
PRINT STATISTICAL PARAMETERS
PRINT CONCENTRATION TABLEAU
IS TT = TL ?
NO
YES
END

FIGURE B-2 FLOW CHART FOR IMPLICIT MODEL

```
      PROGRAM DIFFUI(INPUT, OUTPUT)
      DIMENSION C(120,10,10) ,UD(10), P(120,10), CPER(120, 1), XDI(120),
     1 XB(120,10), CX(120,10), CY(120,10), PSIX(120,10), PSIY(120,10),
     2 ALPH(120,10), XA(120,10), XC(120,10),XS(120,10), YA(120,10),
     3 YB(120,10), YC(120,10), YS(120,10), PREC(10)
      DIMENSION FX(10),XMC(10),CM(10),VXP(10),SD(10),SK(10),PK(10)
      DIMENSION BXP1(10), BXM1(10)
  101 FORMAT (5X,4HIX =,I4,3X,4HIY =,I4,3X,6HTEST = ,F13.10)
  102 FORMAT (2I5,5X,3I5)
  104 FORMAT (5F10.2,F20.0)
  105 FORMAT (I3)
  106 FORMAT (1H1)
  107 FORMAT (40X, 13H GRID SIZE IS, F7.4, 8H FEET BY, F7.4, 5H FEET,
     1 10X, 8H TIME IS,F17.4, 4H SEC/ 20X,31HCENTROID OF DISTRIBUTION IS
     2 AT ,F13.3, 30H FEET   STANDARD DEVIATION IS ,F13.5,5H FEET/1H1)
  108 FORMAT (10F8.0)
  109 FORMAT (18H FAILURE [illegible] ITERM.)
  110 FORMAT (5X,I4,5F18.8 ,5X,F15.8 ,F13.3)
  111 FORMAT (////,50X,15H SUMMARY OF DATA,//,40X,17HGRID INCREMENT IS,
     1F7.4,8H FEET BY,F7.4,5H FEET,/,40X,17HTIME INCREMENT IS,F10.4,9H
     2SECONDS,/,40X,23HTOTAL TIME PROCESSED IS,F17.4,9H  SECONDS,//,40X,
     330HCOEFFICIENTS OF EDDY VISCOSITY,/,50X,5HDX = ,F10.4,23H SQUARE F
     4EET PER SECOND,/,50X,5HDY = ,F10.4,23H SQUARE FEET PER SECOND,//
     5,60X,16HVELOCITY PROFILE,/,50X,5HPOINT,15X,17HVELOCITY (FT/SEC),//
     6(50X,I3,17X,F10.4,/))
  113 FORMAT (1H+,  9X, 1HB, 37X, 1HC, 36X, 1HB)
  114 FORMAT (10X, 1H1, 37X, 1H1, 36X, 1H1,  6X, 13HCUMU PCT CONC , 4X,
 1141 8HDISTANCE )
  116 FORMAT(1H1////33X,58HMATERIAL  INTRODUCED AS AN INSTANTANEOUS LINE
     1SOURCE AT X =  ,I3)
  117 FORMAT(1H1////34X,57HMATERIAL  INTRODUCED AS AN INSTANTANEOUS POINT
     1 SOURCE AT ( ,I3,1H,,I2,1H))
  118 FORMAT(1H1,12X,4HTIME,14X,3HU*T,13X,6HX MEAN,10X,7HSTD DEV,9X,
     1   9HDISP COFF ,10X,4HITER)
  119 FORMAT (//3X,4HTIME,3X,4HITER,3X,7HY POINT,2X,8HMAX CONC,3X,
     18HCENTROID,4X,8HSTAN DEV,5X,8HSKEWNESS,3X,10HPEAKEDNESS,3X,
     29HPRECISION,4X,16HDISPERSION COEFF/ 4X,3HSEC,21X,4HC/CI,8X,2HFT,
     310X,2HFT,34X,5HINDEX,9X,9HFT**2/SEC / F9.2,I4,5X,I3,F13.5,F12.4,
     43F12.5,F13.5,F19.10/(18X,I3,F13.5,F12.4,3F12.5,F13.5,F19.10))
  140 FORMAT (/,5X,24HMULTIPLYING COEFFICIENTS,/,5X,4HGAMX,12X,4HGAMY,
     112X,4HGAMT,12X,2HBY,14X,5HPOINT,11X,4HBXP1,12X,4HBXM1,/,4(2X,
     2F14.10),6X,I3,9X,F14.10,2X,F14.10,/,(70X,I3,9X,F14.10,2X,F14.10))
C
C                         DEFINITIONS FOR INPUT DATA
C            KD1       THE NUMBER OF PROBLEMS TO BE SOLVED
C            DX        DIFFUSION COEFFICIENT, X DIRECTION
C            DY        DIFFUSION COEFFICIENT, Y DIRECTION
C            X         GRID INCREMENT (FEET)
C            T         TIME INCREMENT (SECONDS)
C            TI        PRINTING TIME INCREMENT (SECONDS)
C            TL        TIME AT END OF PROBLEM (SECONDS)
C            LX        NUMBER OF GRID POINTS, X DIRECTION
C            LY        NUMBER OF GRID POINTS, Y DIRECTION
C            IFPTSC    EITHER LINE SOURCE (ZERO) OR PLANE SOURCE (ANY
C                         POSITIVE NUMBER)
C            KCX       LOCATION OF DYE INSERTION, X DIRECTION
C            KCY       LOCATION OF DYE INSERTION, Y DIRECTION
C            UD        ARRAY OF MEAN VELOCITIES IN THE X DIRECTION
C
      TS=0.0000000001  $  TSS=TS*100.  $  SUBT=0.00001 $  TEST=0.001
      READ 105, KD1   $   DO 18 KD2=1,KD1
C        DATA READ IN
      READ 104, DX,DY,X,T,TI,TL   $   READ 102, LX,LY,IFPTSC,KCX,KCY
      READ 108, (UD(K),K=1,LY) $ LT=10 $ LPS=IFPTSC
      DO 1 IY=1,LY $ VXP(IY)=0.$ DO 1 IX=1,LX $ CX(IX,IY)=CY(IX,IY)=0.
    1 C(IX,IY, 1)=+0.0$ Y=X $       TT=0       $ ITERM=2  $ TP=TI
   14 LTM1=LT-1    $   LYM1=LY-1    $   LXM1=LX-1    $   LYM2=LY-2
      LXM2=LX-2
      IF (LPS.EQ.0) 60,61
   60 PRINT 116, KCX   $   DO 12 KK=1,LY
   12 C(KCX,KK,1)=1.0   $   AREA=X    $  GO TO 62
C        PRINTING OF COVER SHEET
```

```
   61 PRINT 117, KCX, KCY    $    C(KCX,KCY,1)=1.0    $    AREA = X*Y
   62 PRINT 111, X,Y,T,TL,DX,DY,((I,UD(I)),I=2,LYM1)
      PRINT 106  $  XDI(1)=(KCX-1)*(-X)  $  DO 63 KX=2,LX
   63 XDI(KX)=XDI(KX-1)+X  $    TT=TS
C          CALCULATION OF COMMONLY USED RELATIONSHIPS
      DO 81 IY=1,LY    $    BXP1(IY)=DX*T/2./X/X-UD(IY)*T/4./X
   81 BXM1(IY)=DX*T/2./X/X+UD(IY)*T/4./X
      GAM=-DX*T/X/X - 0.50     $    BY=DY*T/2./Y/Y
      GAMY=-DY*T/Y/Y-0.50     $  GAMT=GAM +GAMY+2.
      PRINT 140, GAM,GAMY,GAMT,BY,(IY,BXP1(IY),BXM1(IY), IY=2,LYM1)
C          START OF ITERATIVE PROCESS
   44 DO 39 IT=1,LTM1
C          START OF SOLUTION FOR VALUES OF CX
      DO 9 IX=2,LXM1  $  DO 3 IY=2,LYM1
C          CALCULATION OF MATRIX COEFFICIENTS AND OF KNOWN VALUES AT
C          TIME T
      ALPH(IX,IY)=-(GAMT*C(IX,IY,IT)+BXP1(IY)*C(IX+1,IY,IT)
     1   +BXM1(IY)*C(IX-1,IY,IT) + BY*(C(IX,IY-1,IT)+C(IX,IY+1,IT)))
      PSIX(IX,IY)=-(C(IX,IY,IT)*(GAM+2.*GAMY+2.5)+C(IX+1,IY,IT)*BXP1(IY)
     1   +BXM1(IY)*C(IX-1,IY,IT)+2.*BY*(C(IX,IY+1,IT)+C(IX,IY-1,IT)))
      YB(IX,IY)=GAMY    $  XB(IX,IY)=-DX*T/X/X-1.
      YA(IX,IY)=YC(IX,IY)=BY    $    XA(IX,IY)=BXM1(IY)
    3 XC(IX,IY)=BXP1(IY)    $  YB(IX,1)=YB(IX,LY)=-1.0
    9 YC(IX,1)=YA(IX,LY)=1.0  $  DO 82 IY=2,LYM1
      XB(1,IY)=XB(LX,IY)=BXM1(IY)-BXP1(IY) $ PSIX(LX,IY)=-PSIX(LXM1,IY)
      XC(1,IY)=GAM+2.0*BXP1(IY)    $    XA(LX,IY)=-XC(1,IY)
   82 PSIX(1,IY)=PSIX(2,IY)    $    ITER=0
C          SOLUTION OF TRIDIAGONAL MATRIX
   19 DO 76 IY=2,LYM1    $    XS(1,IY)=XC(1,IY)/XB(1,IY)
      PSIX(1,IY)= PSIX(1,IY)/XB(1,IY)    $  DO 2 IX=2,LXM1
      DEM=XB(IX,IY)-XA(IX,IY)*XS(IX-1,IY) $ XS(IX,IY)=XC(IX,IY)/DEM
    2 PSIX(IX,IY)=(PSIX(IX,IY)-XA(IX,IY)*PSIX(IX-1,IY))/DEM
      CX(LX   ,IY)=PSIX(LX   ,IY)=(PSIX(LX   ,IY)-XA(LX   ,IY)*PSIX(LXM1,IY)
     1)/(XB(LX   ,IY)-XA(LX   ,IY)*XS(LXM1,IY))
      DO 4 IX=2,LX    $ KX=LX+1-IX
    4 CX(KX,IY)=PSIX(KX,IY)-XS(KX,IY)*CX(KX+1,IY)
```

```
C         SOLUTION FOR VALUES OF CX IS COMPLETE
   76 CONTINUE
C         START OF SOLUTION FOR VALUES OF CY
      DO 6 IX=2,LXM1 $ DO 8 IY=2,LYM1  $   XB(IX,IY)=GAM
    8 PSIY(IX,IY)=ALPH(IX,IY)-BXP1(IY)*CX(IX+1,IY)-BXM1(IY)*CX(IX-1,IY)
     1   -GAM*CX(IX,IY)
    6 PSIY(IX,1)=PSIY(IX,LY)=0.
      DO 10 IX=2,LXM1  $   YS(IX,1)=YC(IX,1)/YB(IX,1)
C         SOLUTION OF TRIDIAGONAL MATRIX
      PSIY(IX,1)=PSIY(IX,1)/YB(IX,1)  $  DO 7 IY=2,LYM1
      DEM=YB(IX,IY)-YA(IX,IY)*YS(IX,IY-1) $ YS(IX,IY)=YC(IX,IY)/DEM
    7 PSIY(IX,IY)=(PSIY(IX,IY)-YA(IX,IY)*PSIY(IX,IY-1))/DEM
      CY(IX,LY   )=PSIY(IX,LY   )=(PSIY(IX,LY   )-YA(IX,LY   )*PSIY(IX,LYM1)
     1)/(YB(IX,LY   )-YA(IX,LY   )*YS(IX,LYM1))
      DO 10 IY=2,LY     $  KY=LY+1-IY
   10 CY(IX,KY)=PSIY(IX,KY)-YS(IX,KY)*CY(IX,KY+1)
C         SOLUTION FOR VALUES OF CY IS COMPLETE
   24 DO 16 IX=2,LXM1    $   DO 16 IY=2,LYM1$  C(IX,IY,IT+1) = CY(IX,IY)
      IF (CY(IX,IY).LT.0.0) 21,22
   21 C(IX,IY,IT+1)=0.0
   22 IF (IY.EQ.LYM1)25,16
C        --COMPUTATION OF LATERAL BOUNDARY CONDITIONS--
   25 C(IX,1,IT+1) = C(IX,2,IT+1)   $   C(IX,LY,IT+1) = C(IX,LYM1,IT+1)
   26 IF (IX.EQ.LXM1) 27,16
   27 C(1,IY,IT+1) = C(LX,IY,IT+1) = 0.0
C         COMPUTATION OF LONGITUDINAL BOUNDARY CONDITIONS
      IF((C(IX, IY,IT+1).GE.TS) .AND. (C(2, IY,IT+1).GE.TS))29,33
   33 IF((C(IX, IY,IT+1).LT.TS) .AND. (C(2, IY,IT+1).LT.TS))16,34
   34 LM=2   $   IF (C(IX, IY,IT+1).GT.TS) 31,32
   29 DO 28 LM=1,2   $   IF (LM.EQ.1) 31,32
   32 K1=1    $   K2=2    $   K3=3    $   K4=4    $   K5=5    $   GO TO 30
   31 K1=LX   $  K2=LX-1  $  K3=LX-2  $  K4=LX-3  $  K5=LX-4
   30 DC1=C(K3, IY,IT+1)/C(K2, IY,IT+1)
      DC2=C(K4, IY,IT+1)/C(K3, IY,IT+1)
      DC3=C(K5, IY,IT+1)/C(K4, IY,IT+1)
      DC=ABSF(DC1-DC2)+ABSF(DC2-DC3)+DC1
      C(K1, IY,IT+1)=C(K2, IY,IT+1)/DC
   28 CONTINUE
   16 CONTINUE  $  TT=TT+T  $  DO 53 M=2,LYM1  $  VX=SX=PX=XMC(M)=J=N=0.
C        COMPLETION OF CONCENTRATION CALCULATIONS. START CALCULATION OF
C        DISPERSIVE PARAMETERS
      DO 50 KX=1,LX   $   IF (C(KX,M,IT+1).GT.TS) 49,50
   49 XMC(M)=XMC(M)+XDI(KX)*C(KX,M,IT+1)   $   J=J+1   $   JA=KX
   50 CONTINUE  $  JB=JA-J  $  DO 52 KX=JB,JA   $ XST=XDI(KX)-XMC(M)
      TE=XST*C(KX,M,IT+1) $ VX=VX+XST*TE  $  SX=SX+TE*XST**2$IF(N)52,54
   54 CM(M)=0.   $   IF (ABSF(XST).LT.TEST) 51,52
   51 CM(M)=C(KX,M,IT+1)/AREA  $   N=1
   52 PX=PX+TE*XST**3 $ SD(M)=SQRTF(VX) $ SK(M)=SX/SD(M)**3
      PK(M)=PX/SD(M)**4 $ EX(M)=(VX  - VXP(M))/2./T $ VXP(M)=VX
   53 PREC(M)=3.*SK(M)**2-2.*PK(M)+6.
C        PRINTING OF STATISTICAL PARAMETERS.
C                CM = MAXIMUM CONCENTRATION
C               XMC = LOCATION OF CM
C                SD = STANDARD DEVIATION
C                SK = SKEWNESS
C                PK = PEAKEDNESS
C              PREC = PRECISION INDEX
C                EX = DISPERSION COEFFICIENT
      PRINT 119, TT,ITER,(IY,CM(IY),XMC(IY),SD(IY),SK(IY),PK(IY),
     1   PREC(IY),EX(IY), IY=2,LYM1)
      LS=1  $  IF (TT.LT.TI) 40,5
   40 LS=0 $ IF (TT.GE.TP)5,39
    5  CSUM=0.0  $  PRINT 106
      DO 45 KX=1,LX  $  CSUM=CSUM+C(KX, 3,IT+1)  $  DO 45 KY=1,LY
   45 P(KX,KY) = C(KX,KY,IT+1)/AREA $KY=3 $  CSUM=2.*CSUM
      CPER(1,1)=C(1,KY,IT+1)/CSUM*100.  $  DO 46 KX=2,LX
   46 CPER(KX, 1)=(C(KX,KY,IT+1) +C(KX-1,KY,IT+1))/CSUM*100.+CPER(KX-1,
     11)
      PRINT 113 $ PRINT 114  $  KT=IT+1
C        PRINTING OF CONCENTRATION TABLEAU
      PRINT 110, (KX,(P(KX,KY),KY=2,LYM1),CPER(KX, 1),XDI(KX),KX=1,LX)
      PRINT 107,X,Y,TT,XMC(3),SD(3)  $  TP=TP+100.  $  IF(LS)18,39
   39 CONTINUE $ DO 41 IX=1,LX  $  DO 41 IY=1,LY
C        WHEN LT TIME INCREMENTS HAVE BEEN PROCESSED, RETURN TO LT = 1
   41 C(IX,IY,1) = C(IX,IY,LT)  $ GO TO 44
   18 CONTINUE
      END
```

TABLE C-1

NOTATION AND CONVERSION CHARACTERISTIC MODEL

PROGRAM CHDIFF

Input Parameters

FORTRAN Notation	General Notation	Description
DX, DY	E_x, E_y	Turbulent Diffusion Coefficients (ft^2/sec).
X, Y		Spatial Increments (feet)
S		Stability Factor (See Chapter 4)
TI, TP		Printing Time Increment (seconds).
TL		Total Time for Dispersion (seconds).
LX, LY, LT	I,J,K	Number of Grid Points.
LPS		Type of Diffusant Injection Source (Positive Number for Plane Source, Zero for Line Source).
KCX, KCY		Grid Point Location of Tracer Injection Source.
UM		Velocity of Moving Coordinate System (fps).
UD(LY)	u(y)	Velocity Profile over Cross Sections (fps).

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Internal Parameters

T		Time Increment (seconds).
TT		Total Time Processed (seconds).
XDI(LX)		Longitudinal Position of LX with Respect to Dispersant Input Condition.
CHEKX		Maximum Permissible Value of
CHEKT		Maximum Permissible Value of
SAFTY		CHEKT/S
UCK		Lowest Common Multiple of Incremental Velocities.
SD	σ_t	Standard Deviation.
SK		Skewness.
PK		Peakedness.
PREC	P. I.	Precision Index.
EX	E_T	Dispersion Coefficient.
CM	C_{max}	Maximum Concentration.
XMC		Location of CM.
CPER		Cumulative Percent of Concentration Starting from LX=1.
C		Total Concentration in Element of Area
P	C	Concentration in Mass per Unit Area.

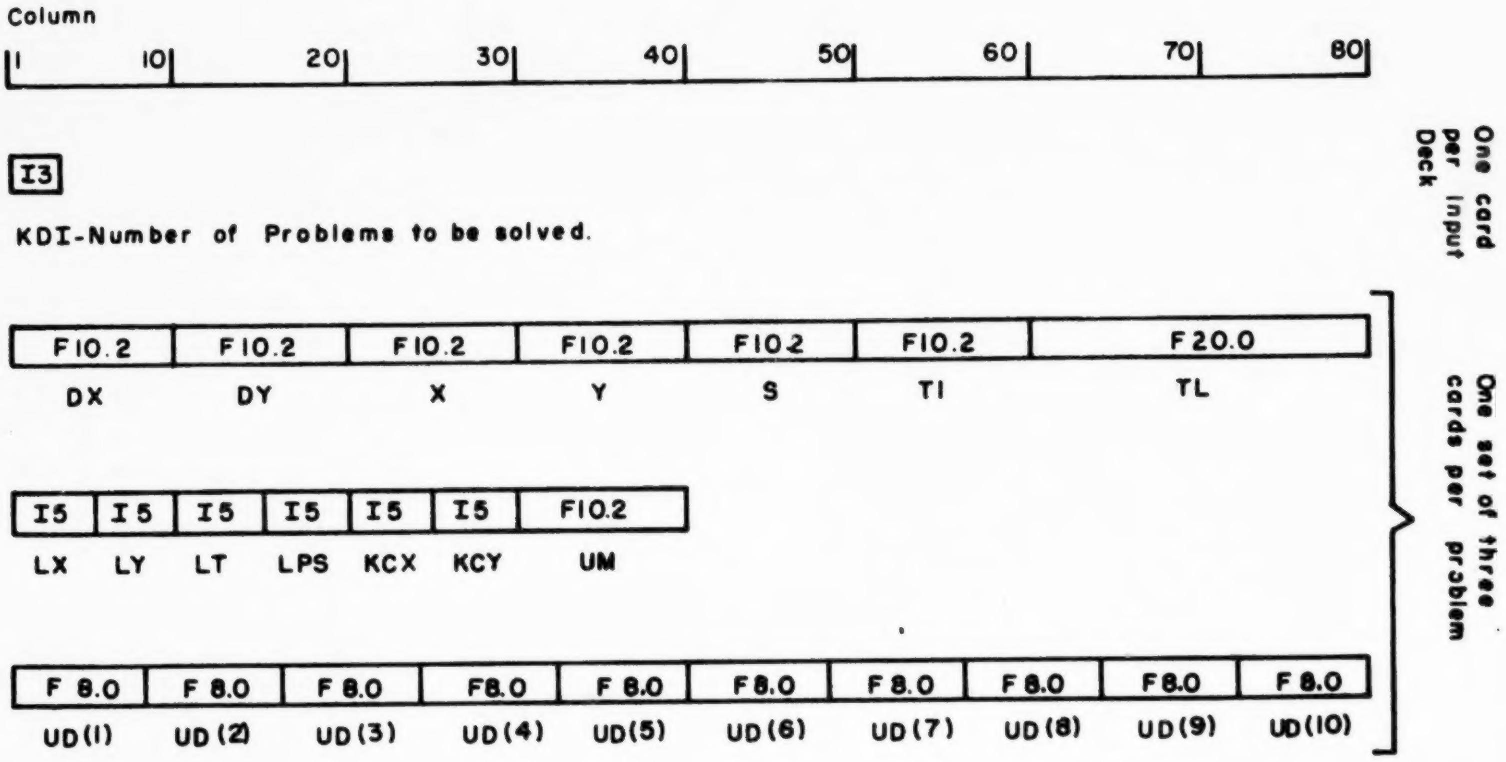

FIGURE C-1

GUIDE FOR DATA INPUT,
CHARACTERISTIC MODEL-PROGRAM CHDIFF

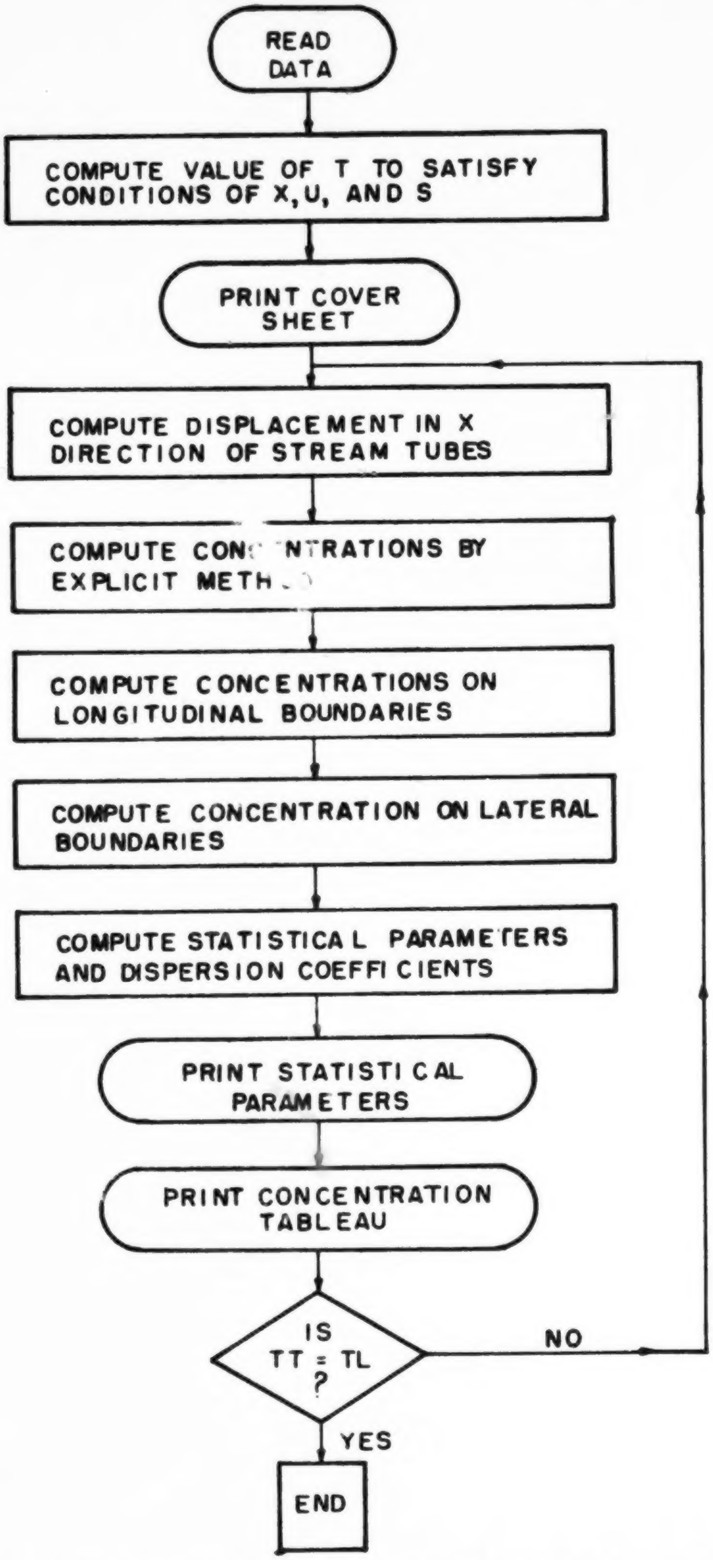
READ DATA
COMPUTE VALUE OF T TO SATISFY CONDITIONS OF X, U, AND S
PRINT COVER SHEET
COMPUTE DISPLACEMENT IN X DIRECTION OF STREAM TUBES
COMPUTE CONCENTRATIONS BY EXPLICIT METHOD
COMPUTE CONCENTRATIONS ON LONGITUDINAL BOUNDARIES
COMPUTE CONCENTRATION ON LATERAL BOUNDARIES
COMPUTE STATISTICAL PARAMETERS AND DISPERSION COEFFICIENTS
PRINT STATISTICAL PARAMETERS
PRINT CONCENTRATION TABLEAU
IS TT = TL ?
NO
YES
END

FIGURE C-2 FLOW CHART FOR CHARACTERISTIC METHOD

```
      PROGRAM CHDIFF (INPUT,OUTPUT)
      DIMENSION C(120,10,10) ,UD(10). P(120,10), CPER(120, 1), XDI(120),
     1 PREC(10),FX(10),XMC(10),CM(10),VXP(10),SD(10),SK(10),PK(10),
     2 DC(20), IDC(10), XI(5), APX(10), APY(3)
  101 FORMAT  (8H CHFKT = ,F15.5,10X. 3HS = ,F7.2,10X,7HSAFTY =,F15.5,
     1  10X,3HT = ,F15.5)
  102 FORMAT (6I5,F10.0)
  104 FORMAT (6F10.2,F20.0)
  105 FORMAT (I3)
  106 FORMAT (1H1)
  107 FORMAT (40X, 13H GRID SIZE IS, F7.4, 8H FEFT BY, F7.4, 5H FEET,
     1 10X, 8H TIME IS,F17.4, 4H SFC/ 20X,31HCENTROID OF DISTRIBUTION IS
     2 AT ,F13.3, 30H FEET   STANDARD DEVIATION IS ,F13.5,5H FEET/1H1)
  108 FORMAT (10F8.0)
  109 FORMAT (17H FAILURF ON ITERM)
  110 FORMAT (5X,I4,7E13.6 ,5X,F15.8 ,F13.3)
  111 FORMAT (////,50X,15HSUMMARY OF DATA,//,40X,17HGRID INCREMENT IS,
     1F7.4,8H FEFT BY,F7.4,5H FEET,/,40X,17HTIME INCREMENT IS,F10.4,9H
     2SECONDS,/,40X,23HTOTAL TIME PROCESSED IS,F17.4,9H  SFCONDS,//,40X,
     330HCOEFFICIENTS OF EDDY VISCOSITY,/,50X,5HDX = ,F10.4,23H SQUARE F
     4FET PER SECOND,/,50X,5HDY = ,F10.4,23H SQUARE FEET PER SECOND,
     5        //,40X,22H~~STABILITY REQUIREMENTS,/~~
     6                      40X,19H  MAXIMUM TIME IS  ,F12.4,8H SECONDS,//
     7,60X,16HVELOCITY PROFILE,/,50X,5HPOINT,15X,17HVELOCITY (FT/SEC),//
     8(50X,I3,17X,F10.4,/))
  113 FORMAT (1H+,  9X, 1HR, 37X, 1HC, 36X, 1HR)
  114 FORMAT (10X, 1H1, 37X, 1H1, 36X, 1H1.  6X, 13HCUMU PCT CONC , 4X,
 1141 8HDISTANCF )
  116 FORMAT(1H1////33X,58HMATERIAL  INTRODUCFD AS AN INSTANTANEOUS LINE
     1SOURCE AT X =  ,I3)
  117 FORMAT(1H1////34X,57HMATERIAL  INTRODUCED AS AN INSTANTANEOUS POINT
     1 SOURCF AT ( ,I3,1H,,I2,1H))
  119 FORMAT (//3X,4HTIMF,3X,4HITER,3X,7HY POINT,2X,8HMAX CONC,9X,
     18HCENTROID,4X,6HSTAN DEV,5X,8HSKFWNESS,3X,10HPFAKEDNESS,3X,
     29HPRECISION,4X,16HDISPERSION COFFF/ 4X,3HSEC,21X,4HC/CI,14X,2HFT,
     310X,2HFT,34X,5HINDEX,9X,9HFT**2/SEC /F9.2,I4,5X,I3,F13.5,A6,F12.4,
     43F12.5,F13.5,F19.10/(18X,I3,F13.5,A6,F12.4,3F12.5,F13.5,F19.10))
C
C                              DEFINITIONS FOR INPUT DATA
C             KD1        THE NUMBER OF PROBLEMS TO BE SOLVED
C             DX         DIFFUSION COEFFICIENT, X DIRECTION
C             DY         DIFFUSION COEFFICIENT, Y DIRECTION
C             X          X DIRECTION GRID INCREMENT (FEET)
C             Y          Y DIRECTION GRID INCREMENT (FEET)
C             S          STABILITY FACTOR
C             TI         PRINTING TIME INCREMENT (SECONDS)
C             TL         TIME AT END OF PROBLEM (SECONDS)
C             LX         NUMBER OF GRID POINTS, X DIRECTION
C             LY         NUMBER OF GRID POINTS, Y DIRECTION
C             LT         NUMBER OF GRID POINTS, T DIRECTION
C             LPS        EITHER LINE SOURCE (ZERO) OR PLANE SOURCE (ANY
C                              POSITIVE NUMBER)
C             KCX        LOCATION OF DYE INSERTION, X DIRECTION
C             KCY        LOCATION OF DYE INSERTION, Y DIRECTION
C             UM         VELOCITY OF GRID SYSTEM
C             UD         ARRAY OF MEAN VELOCITIES IN THE X DIRECTION
C
      DATA APY/6H EXACT,6H APROX,6H       /
      TS=10.**-20.     $  TSS=TS*100.  $   TC = 0.01  $  TCC=.0001
      READ 105, KD1    $   DO 18 KD2=1,KD1
C         DATA READ IN
      READ 104, DX,DY,X,Y,S,TI,TL $   READ 102, LX,LY,LT,LPS,KCX,KCY,UM
      READ 108, (UD(K),K=1,LY)
      LTM1=LT-1    $    LYM1=LY-1    $    LXM1=LX-1 $  LYM2=LY-2
      DO 1 IY=1,LY    $    VXP(IY)=0.    $    DO 1 IX=1,LX
    1 C(IX,IY, 1)=0.0        $ ITER=TT=EXP=0. $ ITERM=50 $ TP=0.
C         CHECK OF PROPER VELOCITY, TIME AND GRID RELATIONSHIP
    6 UCK=100000. $ DO 89 K=2,LYM2 $ UTEM=ABSF(UD(K))
      IF (UTEM.LT.UCK.AND.UTEM.GT.0.0) 88,89
   88 UCK=ABSF(UD(K))
   89 CONTINUE $ DO 91 K=2,LYM2 $ KA=K+1 $ DO 91 KB=KA,LYM1
      UTEM=ABSF(UD(K)-UD(KB))  $  IF (UTEM.LT.UCK.AND.UTEM.GT.0.0) 90,91
   90 UCK=UTEM
   91 CONTINUE $ T=X/UCK  $  CHEKT=(X*Y)**2/2/(DY*Y*Y+DX*X*X)
   92 SAFTY = CHEKT/S  $  IF (SAFTY.GE.T) 14,11
   11 PRINT 101,CHEKT,S,SAFTY,T  $  ITER=ITER+1  $  IF(ITER.GE.ITERM)2,3
    2 PRINT 109  $  GO TO 18
    3 T=T/2.  $  GO TO 92
   14 IF (LPS.EQ.0) 60,61
   60 PRINT 116, KCX   $   DO 12 KK=1,LY
   12 C(KCX,KK,1)=1.0   $   AREA=X    $  GO TO 62
C        PRINTING OF COVER SHEET
   61 PRINT 117, KCX, KCY   $   C(KCX,KCY,1)=1.0   $   AREA = X*Y
   62 PRINT 111, X,Y,T,TL,DX,DY,        CHEKT,((I,UD(I+1)),I=1,LYM2)
      PRINT 106  $  CX=DX*T/X**2  $  CY=DY*T/Y**2  $  TI=TS
   44 DO 39 IT=1,LTM1  $  XDI(1)=(KCX-1)*(-X)+UM*(TI+T)  $ DO 63 KX=2,LX
C        CALCULATION OF DISPLACEMENT OF GRID
   63 XDI(KX)=XDI(KX-1)+X $ DO 83 IY=2,LYM1 $ U=UD(IY)  $ IF(U)95,96
   95 IDC(IY) = U*T/X + (U/ABS(U)*TC)  $  GO TO 97
   96 IDC(IY) = 0
   97 DO 83 IX=2,LXM1 $ IC=IX+IDC(IY) $ IF(IC.GE.1.AND.IC.LE.LX)23,24
C        EXPLICIT COMPUTATION OF CONCENTRATION
   23 C(IC,IY,IT+1) = C(IX,IY,IT)*(1.-2.*CX-2.*CY) +(C(IX+1,IY,IT)
     1  +C(IX-1,IY,IT))*CX + (C(IX,IY+1,IT)+C(IX,IY-1,IT))*CY
   24 IF (IX.EQ.LXM1)25,83
   25 IO = IABS(IDC(IY))+1  $                       IF(UD(IY))71,27,70
C        CALCULATION OF BOUNDARY CONDITIONS FOR STATIONARY GRIDS
   27 C(1,IY,IT+1) = C(LX,IY,IT+1) = 0.0
      IF((C(IX, IY,IT+1).GT.0.) .AND. (C(2. IY,IT+1).GT.0.))29,33
   33 IF((C(IX, IY,IT+1).EQ.0.) .AND. (C(2. IY,IT+1).EQ.0.))83,34
   34 LM=2   $   IF (C(IX, IY,IT+1).GT.0.) 31,32
   29 DO 28 LM=1,2   $   IF (LM.EQ.1) 31,32
   32 K1=1    $    K2=2    $    K3=3    $    K4=4    $    K5=5   $   GO TO 30
   31 K1=LX   $  K2=LX-1   $  K3=LX-2   $  K4=LX-3  $  K5=LX-4
   30 DC1=C(K3, IY,IT+1)/C(K2, IY,IT+1)
      DC2=C(K4, IY,IT+1)/C(K3, IY,IT+1)
      DC3=C(K5, IY,IT+1)/C(K4, IY,IT+1)
      DC=ABSF(DC1-DC2)+ABSF(DC2-DC3)+DC1
      C(K1, IY,IT+1)=C(K2, IY,IT+1)/DC
   28 CONTINUE   $   GO TO 83
C        CALCULATION OF BOUNDARY CONDITIONS FOR MOVING GRID SYSTEM
   70 KE=1 $ K1=IQ $ K2=K1+1 $ K3=K2+1 $ K4=K3+1 $ K5=K4+1 $ GO TO 72
   71 KE=LX $ K1=LX-IQ+1 $ K2=K1-1 $ K3=K2-1 $ K4=K3-1 $ K5=K4-1
   72 IF(C(K2,IY,IT+1).GT.0.) 73,78
   73 DCX=C(K3, IY,IT+1)/C(K2, IY,IT+1)
      DCY=C(K4, IY,IT+1)/C(K3, IY,IT+1)
      DCZ=C(K5, IY,IT+1)/C(K4, IY,IT+1)
      DC(1)=DCZ-DCY  $  DC(2)=DCY-DCX  $  DCC=DCX  $  IF(KE.GT.2)74,76
   74 DO 75 N=1,IQ $ DC(N+2)=ABSF(DC(N))+ABSF(DC(N+1)) $ DCC=DCC+DC(N+2)
   75 C(K2+N,IY,IT+1)=C(K3+N,IY,IT+1)/DCC  $  GO TO 83
   76 DO 77 N=1,IQ $ DC(N+2)=ABSF(DC(N))+ABSF(DC(N+1)) $ DCC=DCC+DC(N+2)
   77 C(K2-N,IY,IT+1)=C(K3-N,IY,IT+1)/DCC  $  GO TO 83
   78 IF (KE.GT.2) 79,81
   79 DO 80 IN=1,IQ
   80 C(K2+IN,IY,IT+1)=0.0  $  GO TO 83
   81 DO 82 IN=1,IQ
   82 C(    IN,IY,IT+1)=0.0
   83 CONTINUE   $   DO 16 IX=1,LX
   84 C(IX,1,IT+1) = C(IX,2,IT+1)  $  C(IX,LY,IT+1) = C(IX,LYM1,IT+1)
   16 CONTINUE  $  TT=TT+T  $  DO 59 M=2,LYM1  $  VX=SX=PX=XMC(M)=J=N=0.
C        COMPLETION OF CONCENTRATION CALCULATIONS. START CALCULATION OF
C        DISPERSIVE PARAMETERS
      DO 50 KX=1,LX   $   IF (C(KX,M,IT+1).GT.TS) 49,50
   49 XMC(M)=XMC(M)+XDI(KX)*C(KX,M,IT+1)   $   J=J+1   $   JA=KX
   50 CONTINUE  $  IF(J.LE.1)GO TO 57
                  JB=JA-J  $  DO 52 KX=JB,JA   $ XST=XDI(KX)-XMC(M)
      TE=XST*C(KX,M,IT+1) $ VX=VX+XST*TE  $  SX=SX+TE*XST**2$IF(N)52,54
   54 CM(M)=0.   $   IF (ABSF(XST).LT.TCC ) 51,52
   51 CM(M)=C(KX,M,IT+1)/AREA  $   N=1 $APX(M)=APY(1)
   52 PX=PX+TE*XST**3 $ SD(M)=SQRTF(VX) $ SK(M)=SX/SD(M)**3
      PK(M)=PX/SD(M)**4 $ EX(M)=(VX  - VXP(M))/2./T $ VXP(M)=VX
      PREC(M)=3.*SK(M)**2-2.*PK(M)+6. $IF(N)59,53
   53 XTT=100000. $ DO 56 KX=1,LX $ XT=XDI(KX)-XMC(M)
      IF (XT.LT.XTT.AND.XT.GT.0.)55,56
   55 XTT=XT $ JB=KX+1 $ JA=KX-2
   56 CONTINUE  $  LD=0 $ DO 67 LA=JA,JB $ LD=LD+1 $ XI(LD)=1.
      DO 66 LB=JA,JB  $   IF (LB-LA)64,65,64
   64 XI(LD+1)=((XMC(M)-XDI(LB))/(XDI(LA)-XDI(LB)))*XI(LD) $ GO TO 66
   65 XI(LD+1)=XI(LD)
   66 CONTINUE  $  XIT=XI(LD+1)*C(LA,M,IT+1)/AREA  $  LD=0
   67 CM(M)=CM(M)+XIT  $  APX(M)=APY(2)  $   GO TO 59
   57 CM(M)=XMC(M)=SD(M)=SK(M)=PK(M)=PREC(M)=EX(M)=0.0 $ APX(M)=APY(3)
   59 CONTINUE
C        PRINTING OF STATISTICAL PARAMETERS.
C                CM = MAXIMUM CONCENTRATION
C               XMC = LOCATION OF CM
C                SD = STANDARD DEVIATION
C                SK = SKEWNESS
C                PK = PEAKEDNESS
C              PREC = PRECISION INDEX
C                FX = DISPERSION COEFFICIENT
      PRINT 119,TT,ITER,(IY,CM(IY),APX(IY),XMC(IY),SD(IY),SK(IY),PK(IY),
     1   PREC(IY),FX(IY), IY=2,LYM1)
      LS=1  $  IF (TT.LT.TL) 40,5
   40 LS=0 $ IF (TT.GE.TP)5,39
    5  CSUM=0.0  $  PRINT 106
      DO 45 KX=1,LX  $  CSUM=CSUM+C(KX, 4,IT+1)  $  DO 45 KY=1,LY
   45 P(KX,KY) = C(KX,KY,IT+1)/AREA $KY=4 $  CSUM=2.*CSUM
      CPER(1,1)=C(1,KY,IT+1)/CSUM*100.  $  DO 46 KX=2,LX
   46 CPER(KX, 1)=(C(KX,KY,IT+1) +C(KX-1,KY,IT+1))/CSUM*100.+CPER(KX-1,
     11)
      PRINT 113 $ PRINT 114  $  KT=IT+1
C        PRINTING OF CONCENTRATION TABLEAU
      PRINT 110, (KX,(P(KX,KY),KY=1,LY  ),CPER(KX, 1),XDI(KX),KX=1,LX)
      PRINT 107,X,Y,TT,XMC(4),SD(4)  $  TP=T          $  IF(LS)18,39
   39 CONTINUE $ DO 41 IX=1,LX  $  DO 41 IY=1,LY
C        WHEN LT TIME INCREMENTS HAVE BEEN PROCESSED, RETURN TO LT = 1
   41 C(IX,IY,1) = C(IX,IY,LT)  $ GO TO 44
   18 CONTINUE
      END
```